LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060622\
Data File : BF128696.D
Acq On : 06 Jun 2022 15:00
Operator : CG\JU
Sample : N3113-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-346

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-BF060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128696.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.387	183	187	200	rBV	41651	80136	2.85%	0.418%
2	5.046	465	469	475	rVB	35100	40689	1.45%	0.212%
3	5.481	539	543	558	rVB	2550709	2507172	89.29%	13.084%
4	6.493	711	715	725	rBV	2814128	2556438	91.04%	13.341%
5	6.563	725	727	730	rVB	46977	36130	1.29%	0.189%
6	6.822	767	771	774	rBV	712257	553905	19.73%	2.891%
7	7.387	861	867	870	rBV	1666183	1614720	57.50%	8.426%
8	8.104	984	989	992	rBV	737305	642819	22.89%	3.355%
9	9.186	1167	1173	1176	rBV	2930985	2807985	100.00%	14.653%
10	9.863	1280	1288	1291	rBV	853641	727873	25.92%	3.798%
11	10.657	1418	1423	1426	rBV	1809245	1601244	57.02%	8.356%
12	11.351	1537	1541	1543	rBV	756597	669117	23.83%	3.492%
13	11.369	1543	1544	1548	rVB	125380	92789	3.30%	0.484%
14	11.745	1604	1608	1611	rBV	98593	85587	3.05%	0.447%
15	11.880	1628	1631	1637	rBV2	235019	218598	7.78%	1.141%
16	11.963	1642	1645	1647	rBV2	29113	30661	1.09%	0.160%
17	12.451	1722	1728	1731	rBV2	117819	114426	4.08%	0.597%
18	12.563	1744	1747	1750	rVB	174950	145757	5.19%	0.761%
19	12.669	1761	1765	1771	rBV	118661	136344	4.86%	0.712%
20	12.792	1777	1786	1788	rBV	147587	154645	5.51%	0.807%
21	12.939	1807	1811	1814	rBV	2369503	2026395	72.17%	10.575%
22	13.510	1903	1908	1912	rBV3	30637	45103	1.61%	0.235%
23	13.839	1961	1964	1966	rBV2	34516	34387	1.22%	0.179%
24	13.874	1966	1970	1982	rVB5	56186	151839	5.41%	0.792%
25	13.992	1982	1990	1993	rBV	577610	592414	21.10%	3.091%
26	14.016	1993	1994	2001	rVB	101695	75813	2.70%	0.396%
27	14.092	2001	2007	2012	rBV	323934	355483	12.66%	1.855%
28	14.469	2067	2071	2074	rVB3	38579	40844	1.45%	0.213%
29	14.774	2120	2123	2126	rVB	29253	29553	1.05%	0.154%
30	15.027	2162	2166	2170	rBV	73038	123770	4.41%	0.646%
31	15.110	2176	2180	2182	rBV2	41641	45366	1.62%	0.237%
32	15.327	2214	2217	2224	rVB	46659	66902	2.38%	0.349%
33	15.392	2224	2228	2234	rBV	64961	78304	2.79%	0.409%
34	15.457	2234	2239	2243	rBV2	393155	490274	17.46%	2.558%
35	15.486	2243	2244	2250	rVB4	45585	50669	1.80%	0.264%
36	15.927	2315	2319	2323	rVB2	34646	44368	1.58%	0.232%

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Misc :
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Integration Parameters: rteint.p
Integrator: RTE
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Start Thrs: 0.2 Max Peaks: 100
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.904	2480	2485	2491	rVB4	24746	56363	2.01%	0.294%
38	17.339	2556	2559	2567	rVB3	20237	37912	1.35%	0.198%

Sum of corrected areas: 19162794

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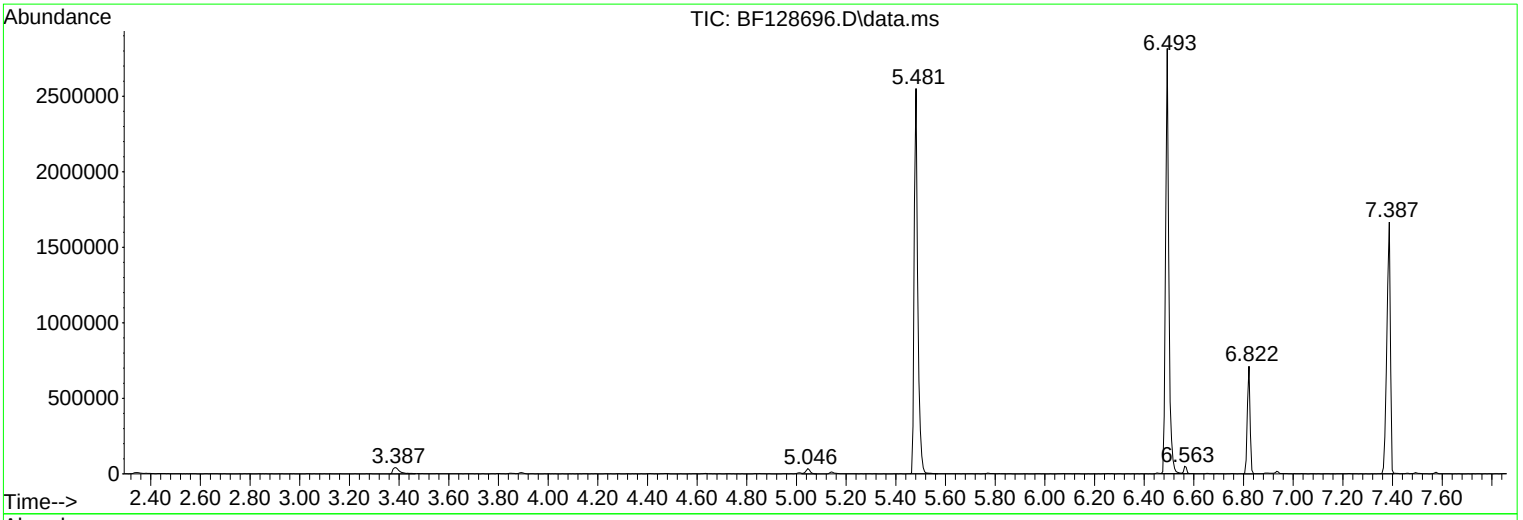
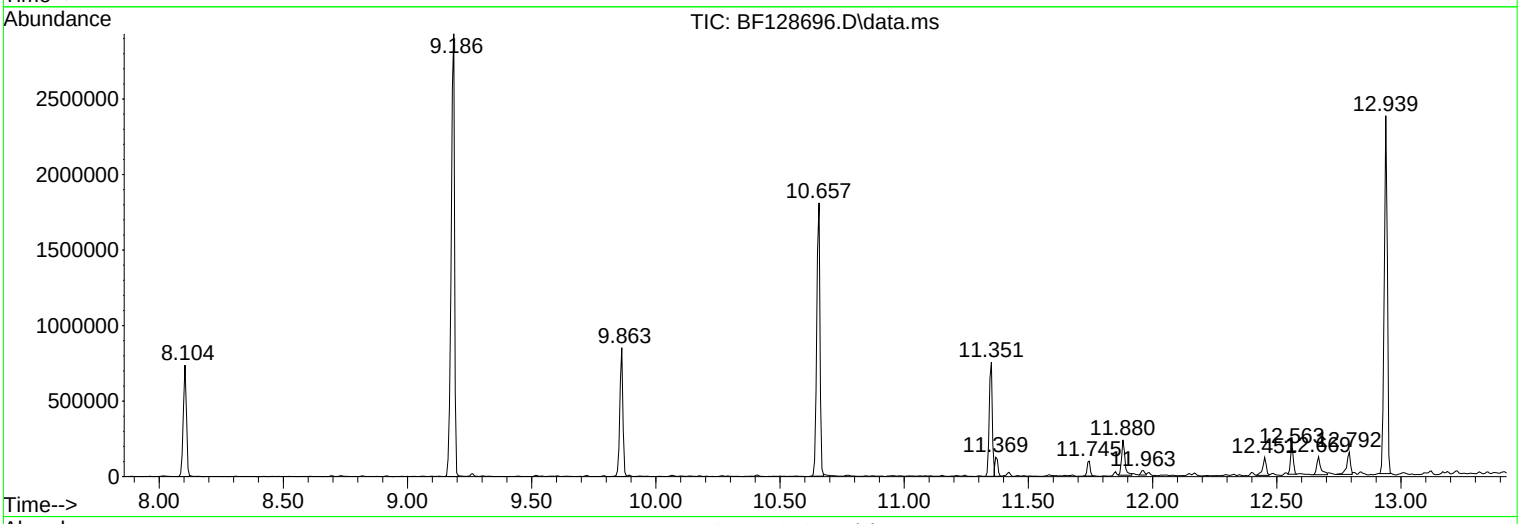
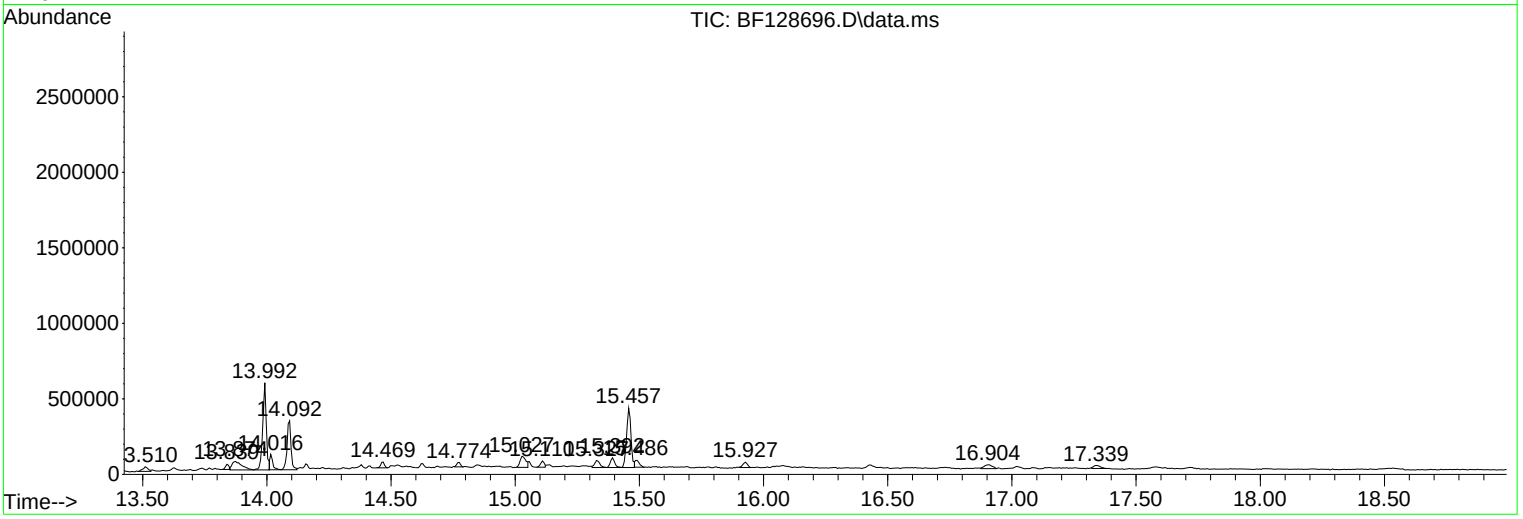
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Sample : N3113-03
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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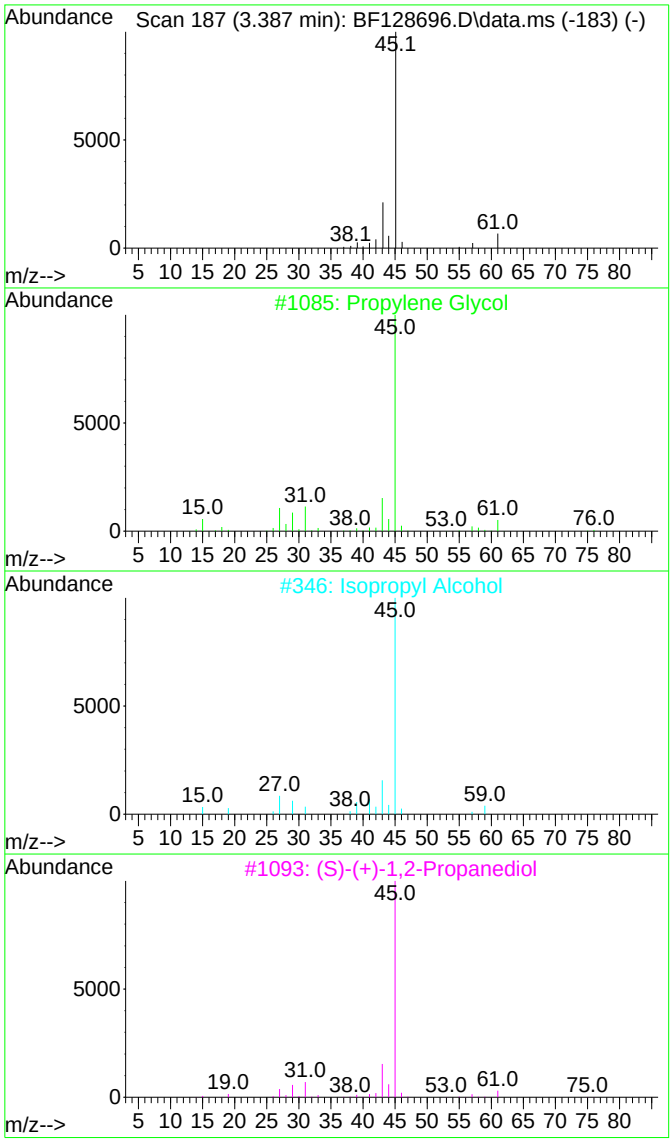
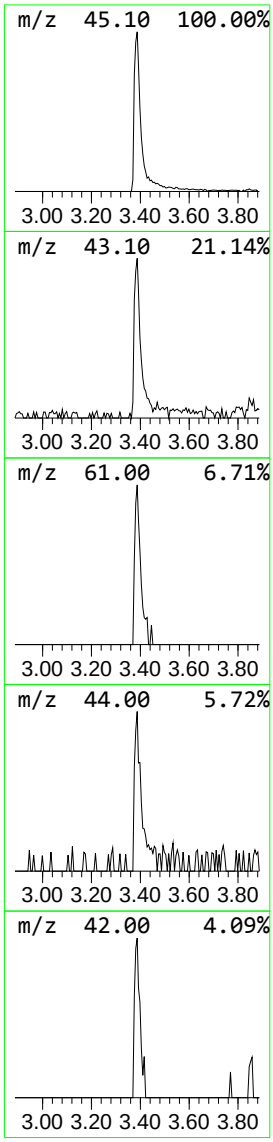
Peak Number 1 unknown3.387 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.387	2.89 ng	80136	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	9
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5	Formamide	45	CH3NO	000075-12-7	5





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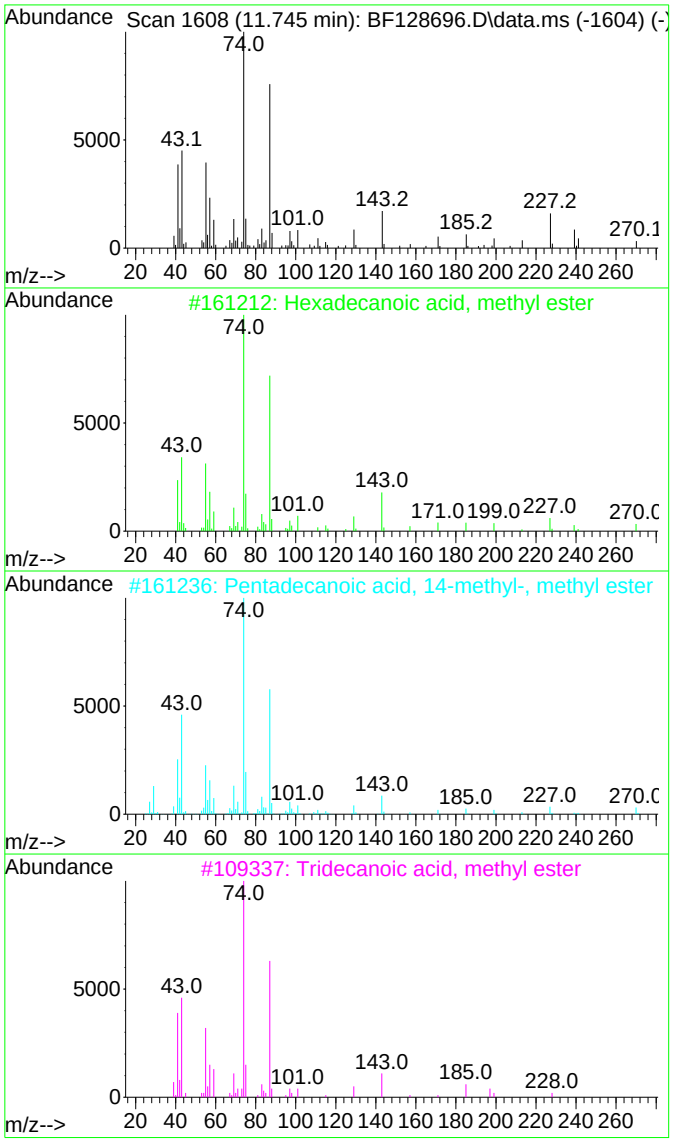
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

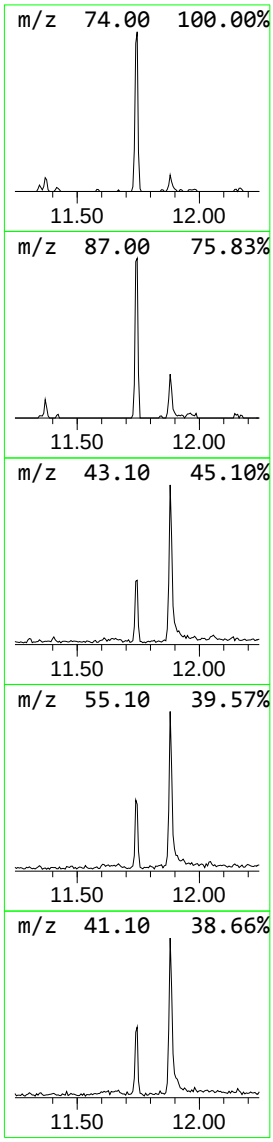
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.745	2.56 ng	85587	Phenanthrene-d10	11.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4	Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	83
5	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	83





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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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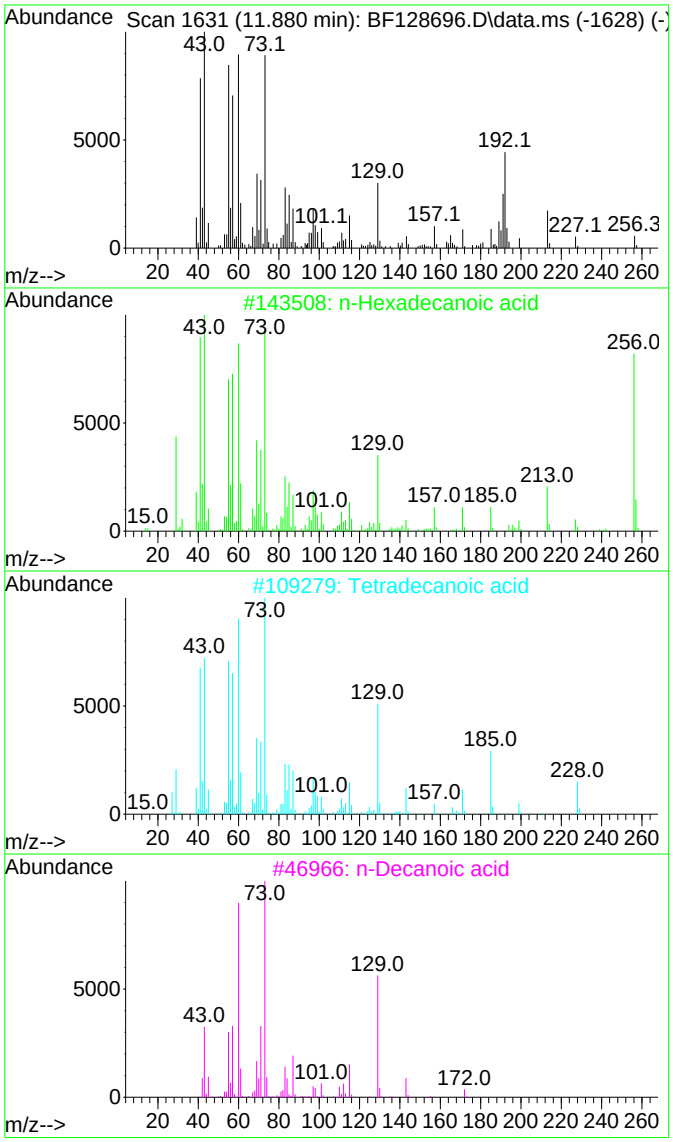
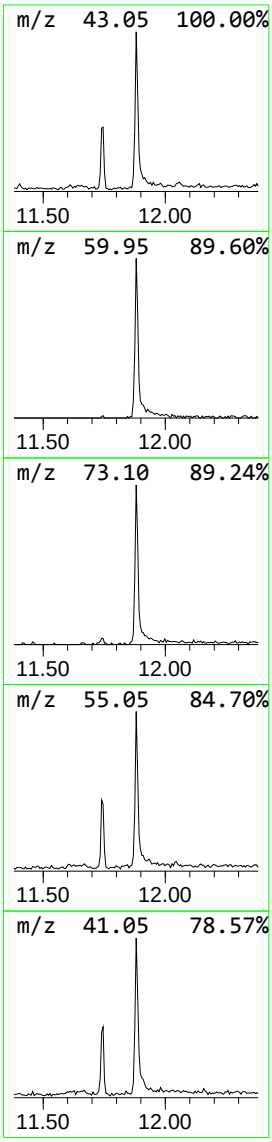
Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	6.53 ng	218598	Phenanthrene-d10	11.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	n-Decanoic acid	172	C10H20O2	000334-48-5	86
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	60
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





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TIC Library : C:\Database\NIST20.L
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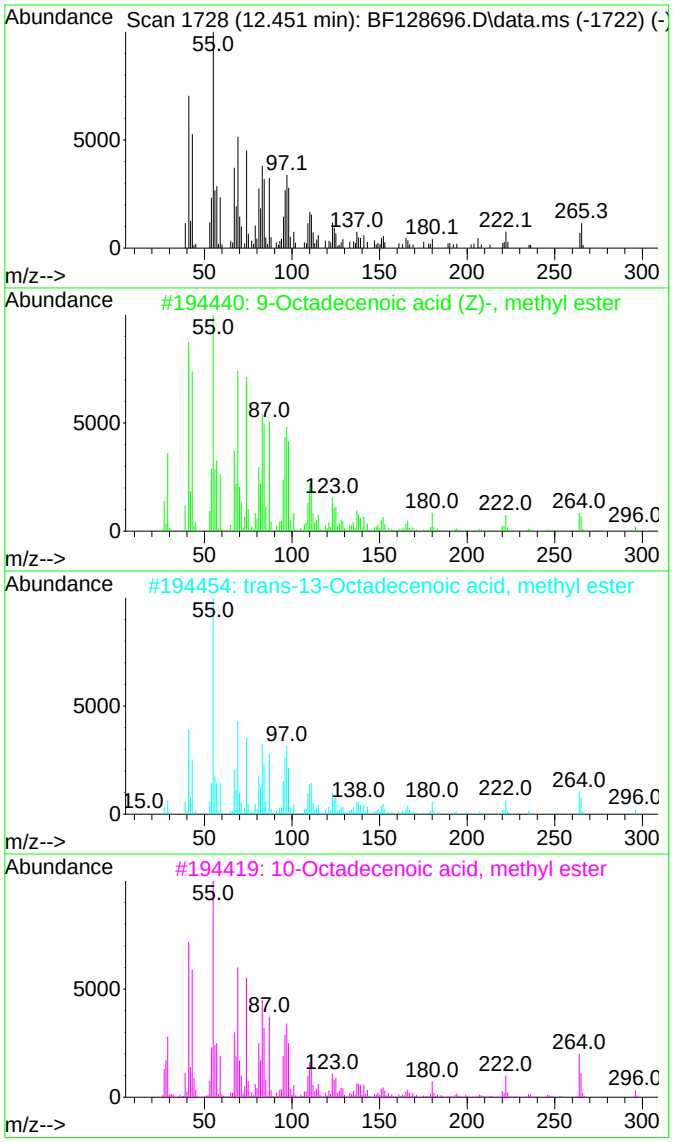
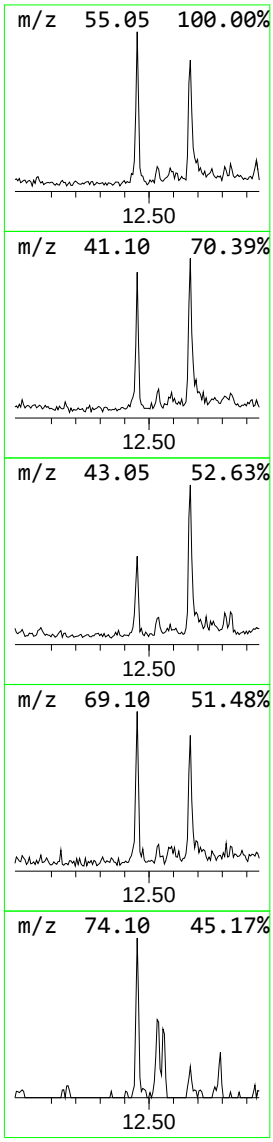
****
Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.451	3.42 ng	114426	Phenanthrene-d10	11.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	90
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	90
4	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	83
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	83





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TIC Library : C:\Database\NIST20.L
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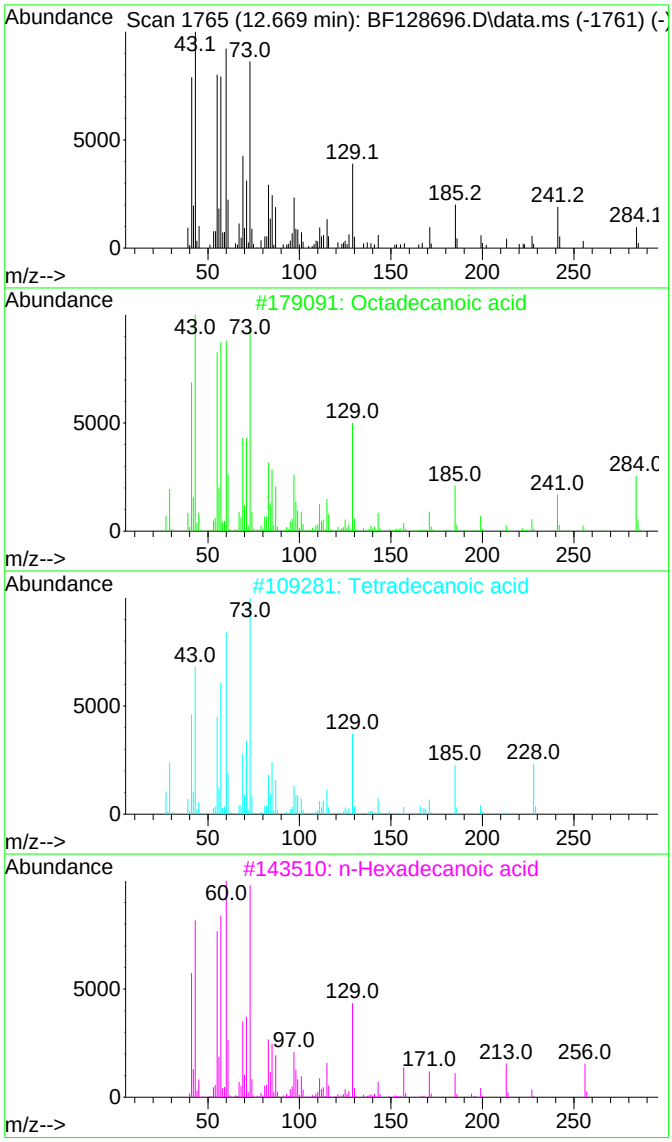
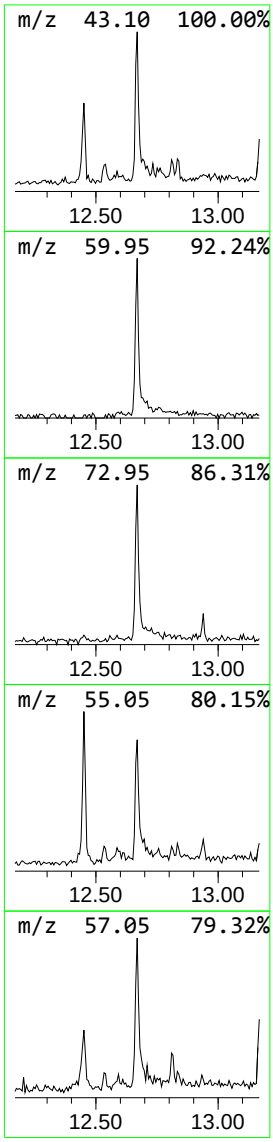
Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.669	4.08 ng	136344	Phenanthrene-d10	11.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	59





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TIC Library : C:\Database\NIST20.L
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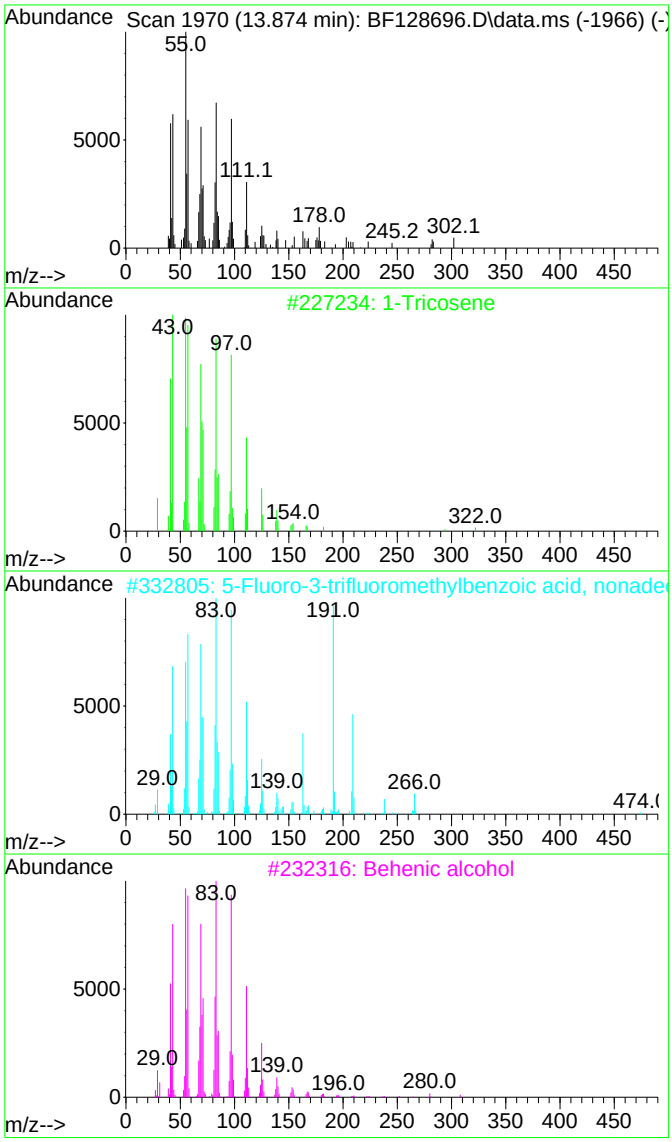
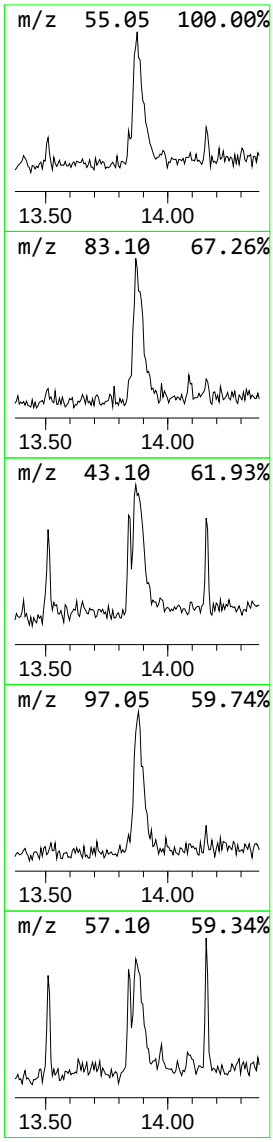
Peak Number 6 1-Tricosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	5.13 ng	151839	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	93
2	5-Fluoro-3-trifluoromethylbenzoi...	474	C27H42F4O2	1000338-91-1	87
3	Behenic alcohol	326	C22H46O	000661-19-8	87
4	hexadecyl acrylate	296	C19H36O2	013402-02-3	83
5	1-Docosene	308	C22H44	001599-67-3	74





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TIC Library : C:\Database\NIST20.L
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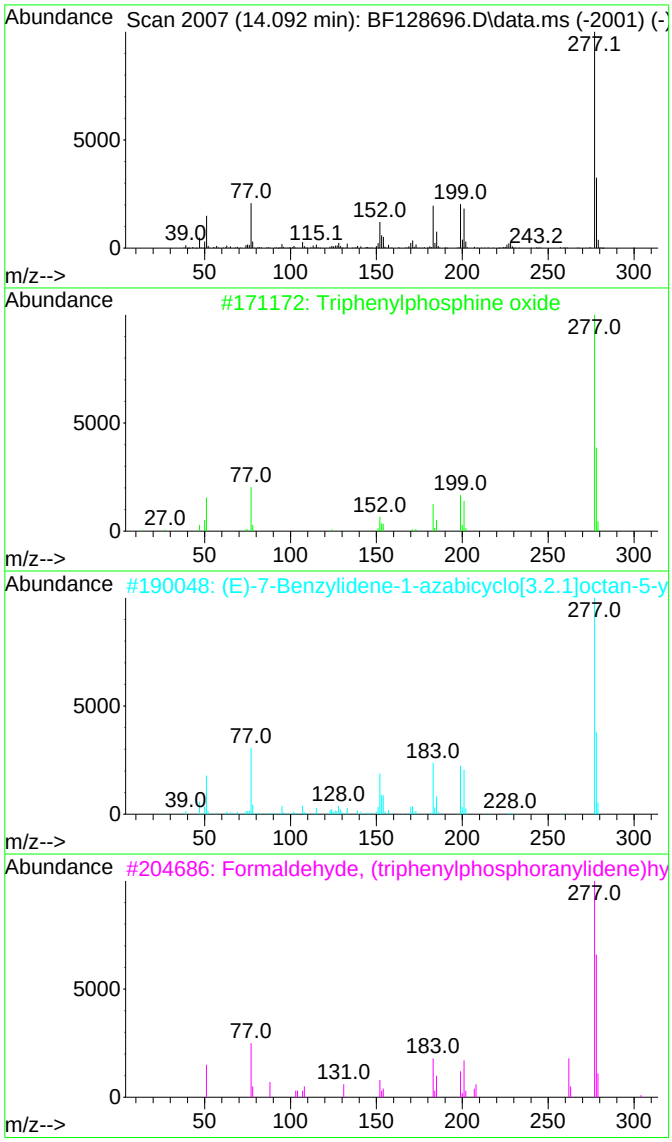
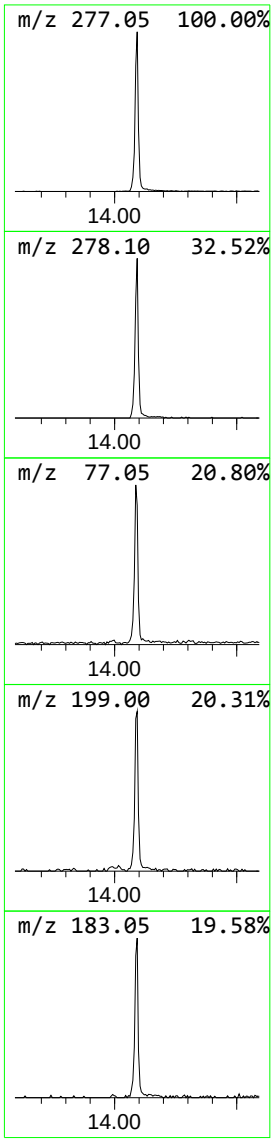
Peak Number 7 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.092	12.00 ng	355483	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	90
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	43
5	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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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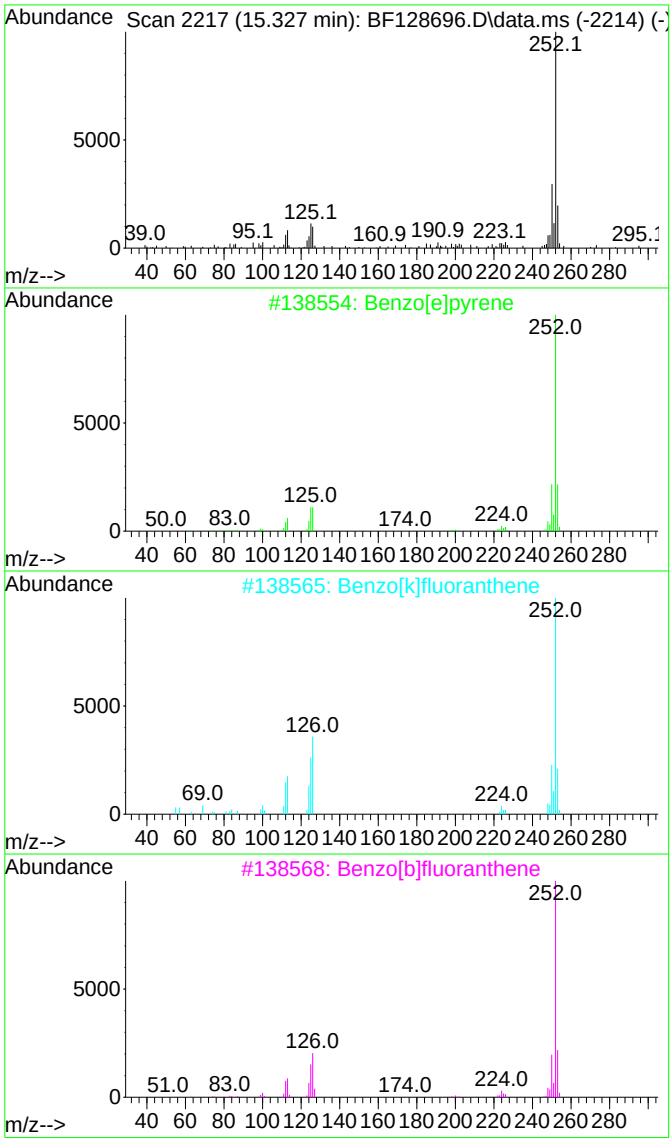
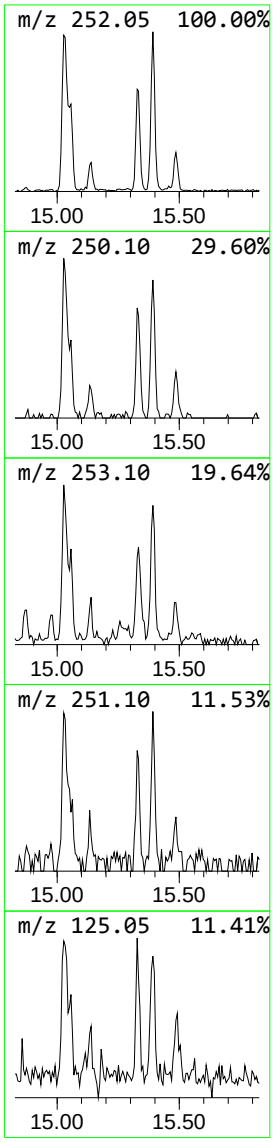
Peak Number 8 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.327	2.73 ng	66902	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4	Perylene	252	C20H12	000198-55-0	90
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	86





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown3.387	3.387	2.9	ng	80136	1	6.822	553905	20.0
Hexadecanoic ac...	11.745	2.6	ng	85587	4	11.351	669117	20.0
n-Hexadecanoic ...	11.880	6.5	ng	218598	4	11.351	669117	20.0
9-Octadecenoic ...	12.451	3.4	ng	114426	4	11.351	669117	20.0
Octadecanoic acid	12.669	4.1	ng	136344	4	11.351	669117	20.0
1-Tricosene	13.874	5.1	ng	151839	5	13.992	592414	20.0
Triphenylphosph...	14.092	12.0	ng	355483	5	13.992	592414	20.0
Benzo[e]pyrene	15.327	2.7	ng	66902	6	15.457	490274	20.0