LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136746.D
Acq On : 27 Dec 2023 05:18
Operator : CG\JU
Sample : 05463-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-11162023

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136746.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	13	17	27	rVB	19320	27844	1.95%	0.224%
2	5.022	492	499	508	rVB	103504	132327	9.26%	1.064%
3	5.434	564	569	572	rBV	1541854	1428344	100.00%	11.482%
4	6.434	734	739	742	rBV	1471616	1353910	94.79%	10.884%
5	6.616	767	770	775	rBV	20940	26963	1.89%	0.217%
6	6.781	795	798	802	rBV	396598	337298	23.61%	2.711%
7	7.345	889	894	897	rBV	984090	812486	56.88%	6.531%
8	8.057	1010	1015	1019	rBV	428936	392858	27.50%	3.158%
9	8.351	1057	1065	1067	rBV8	14222	22299	1.56%	0.179%
10	8.481	1084	1087	1089	rBV	28072	23405	1.64%	0.188%
11	9.080	1186	1189	1194	rBV2	45841	41067	2.88%	0.330%
12	9.139	1194	1199	1202	rBV	1651392	1331063	93.19%	10.700%
13	9.216	1208	1212	1215	rBV3	26650	31401	2.20%	0.252%
14	9.257	1215	1219	1230	rVB	477743	453225	31.73%	3.643%
15	9.539	1262	1267	1270	rVB2	40403	41997	2.94%	0.338%
16	9.675	1288	1290	1294	rBV2	21105	22530	1.58%	0.181%
17	9.816	1307	1314	1317	rBV	449093	365881	25.62%	2.941%
18	9.851	1317	1320	1322	rVB	22011	18302	1.28%	0.147%
19	10.022	1344	1349	1354	rVB4	18073	25589	1.79%	0.206%
20	10.363	1405	1407	1413	rBV	20099	21803	1.53%	0.175%
21	10.610	1445	1449	1453	rBV	857815	706287	49.45%	5.678%
22	10.739	1467	1471	1473	rVB5	15579	19908	1.39%	0.160%
23	10.916	1494	1501	1503	rBV4	12089	21921	1.53%	0.176%
24	11.204	1547	1550	1554	rVB	21156	21813	1.53%	0.175%
25	11.310	1564	1568	1570	rBV	471388	384323	26.91%	3.089%
26	11.333	1570	1572	1575	rVV	190058	148283	10.38%	1.192%
27	11.380	1577	1580	1584	rVB	48173	49694	3.48%	0.399%
28	11.545	1605	1608	1610	rBV	17773	15917	1.11%	0.128%
29	11.704	1633	1635	1637	rBV	18609	15992	1.12%	0.129%
30	11.816	1650	1654	1656	rBV	31459	33873	2.37%	0.272%
31	11.845	1656	1659	1664	rVV	220838	201496	14.11%	1.620%
32	11.921	1669	1672	1675	rVV	56251	67337	4.71%	0.541%
33	11.951	1675	1677	1679	rVB	24521	19553	1.37%	0.157%
34	12.098	1696	1702	1706	rBV4	33346	58183	4.07%	0.468%
35	12.139	1706	1709	1712	rVB2	23836	24072	1.69%	0.194%
36	12.368	1744	1748	1750	rBV	28237	31086	2.18%	0.250%

LSC Area Percent Report

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Instrument :
BNA_F
ClientSampleId :
NB-08-11162023

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.416	1750	1756	1759	rVV5	65855	102621	7.18%	0.825%
38	12.451	1760	1762	1767	rVB2	21883	23918	1.67%	0.192%
39	12.527	1772	1775	1778	rVV	399505	336509	23.56%	2.705%
40	12.563	1778	1781	1785	rVV5	32883	53204	3.72%	0.428%
41	12.633	1789	1793	1796	rVV2	70372	79063	5.54%	0.636%
42	12.680	1799	1801	1804	rVV2	24038	29037	2.03%	0.233%
43	12.757	1808	1814	1820	rVV	326422	371246	25.99%	2.984%
44	12.810	1820	1823	1827	rVB3	18113	27158	1.90%	0.218%
45	12.880	1832	1835	1836	rBV2	18756	22173	1.55%	0.178%
46	12.904	1836	1839	1843	rVV	1570828	1399520	97.98%	11.250%
47	12.980	1848	1852	1856	rBV2	29754	45571	3.19%	0.366%
48	13.063	1864	1866	1867	rBV2	24545	18917	1.32%	0.152%
49	13.086	1868	1870	1874	rVB	51487	50632	3.54%	0.407%
50	13.157	1880	1882	1884	rVB	36378	26405	1.85%	0.212%
51	13.192	1884	1888	1892	rBV2	33340	45155	3.16%	0.363%
52	13.315	1907	1909	1911	rBV2	22207	16209	1.13%	0.130%
53	13.480	1935	1937	1940	rBV2	24069	23812	1.67%	0.191%
54	13.598	1955	1957	1964	rVB	23377	29580	2.07%	0.238%
55	13.710	1974	1976	1979	rBV2	25344	23404	1.64%	0.188%
56	13.815	1991	1994	1996	rVB	40135	36431	2.55%	0.293%
57	13.962	2014	2019	2022	rBV2	379969	447751	31.35%	3.599%
58	13.992	2022	2024	2027	rVB	116123	90863	6.36%	0.730%
59	15.015	2194	2198	2201	rBV	91779	143009	10.01%	1.150%
60	15.380	2257	2260	2265	rVB	76510	96932	6.79%	0.779%
61	15.445	2268	2271	2275	rVV	146422	170391	11.93%	1.370%

Sum of corrected areas: 12439841

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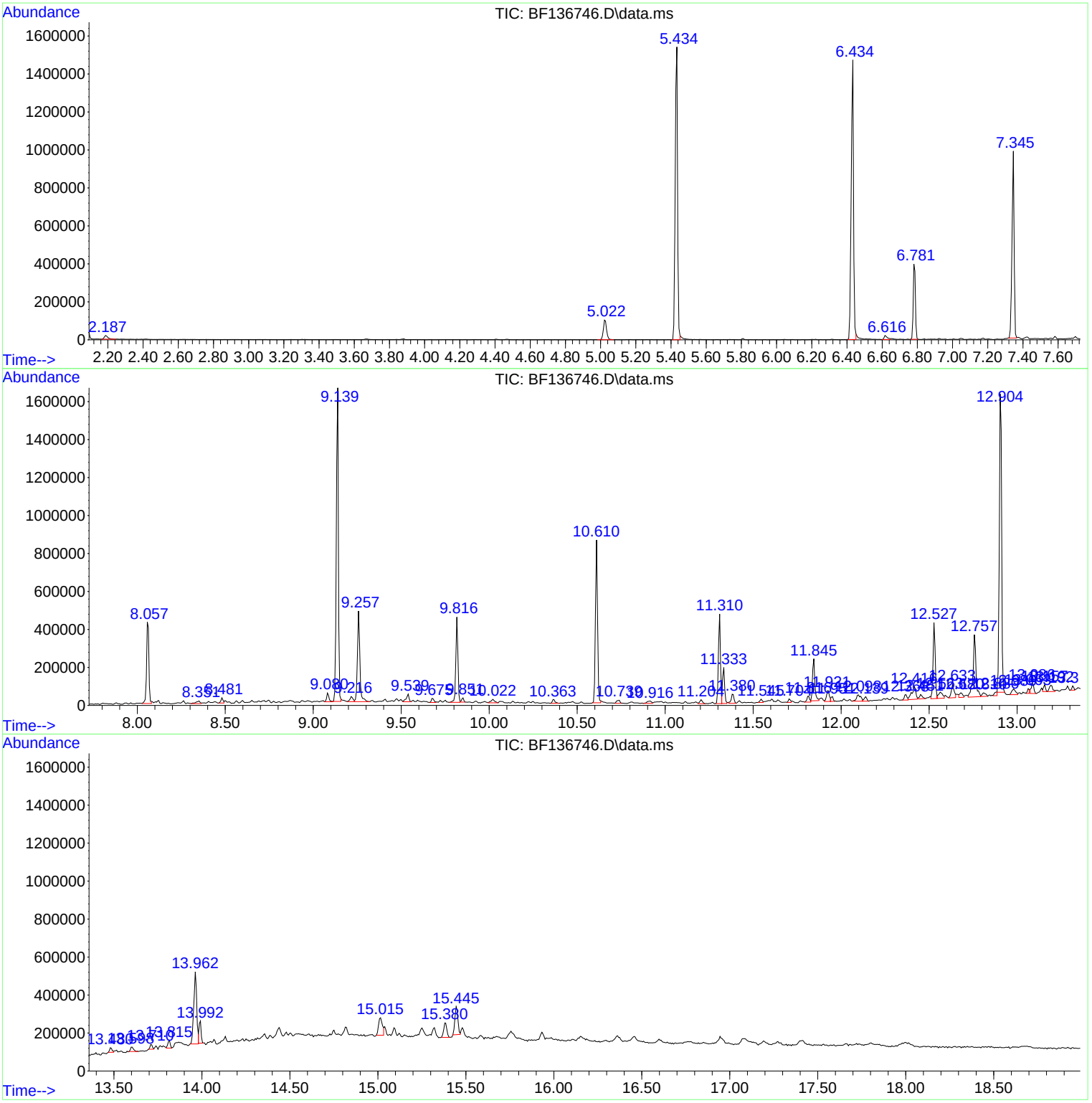
Instrument :
BNA_F
ClientSampleId :
NB-08-11162023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136746.D
Acq On : 27 Dec 2023 05:18
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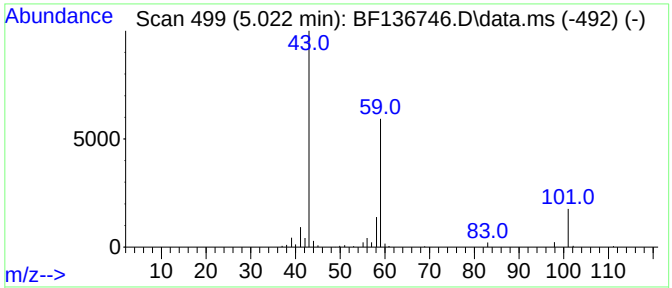
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

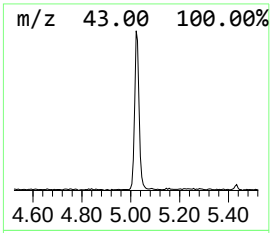
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

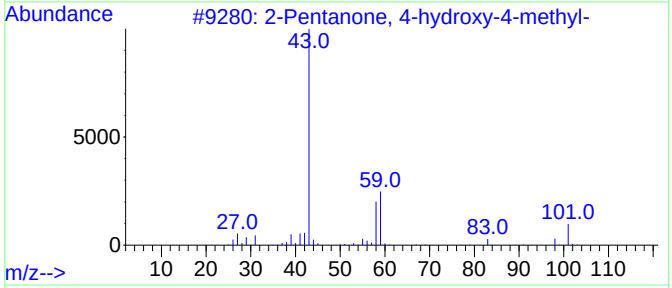
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

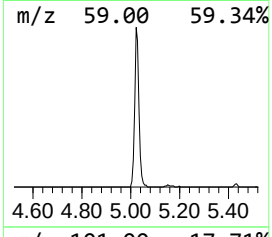
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	7.85 ng	132327	1,4-Dichlorobenzene-d4	6.781

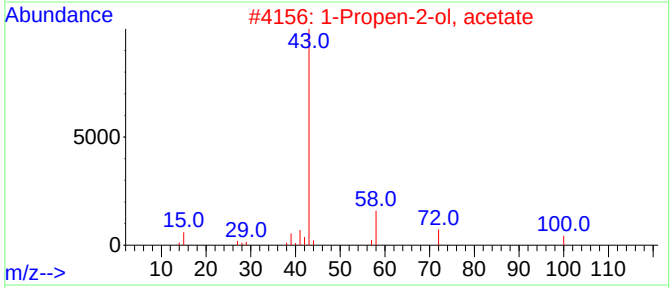
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
3	Butane	58	C4H10	000106-97-8	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Allyl acetate	100	C5H8O2	000591-87-7	9

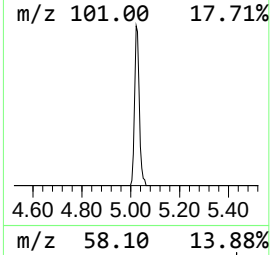


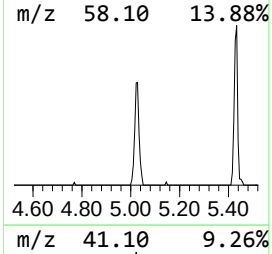


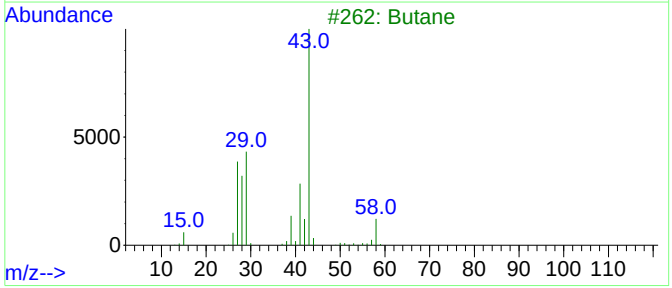


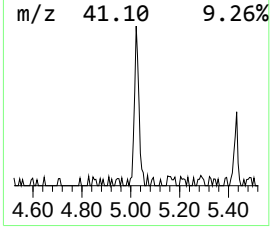












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136746.D
Acq On : 27 Dec 2023 05:18
Operator : CG\JU
Sample : 05463-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-11162023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

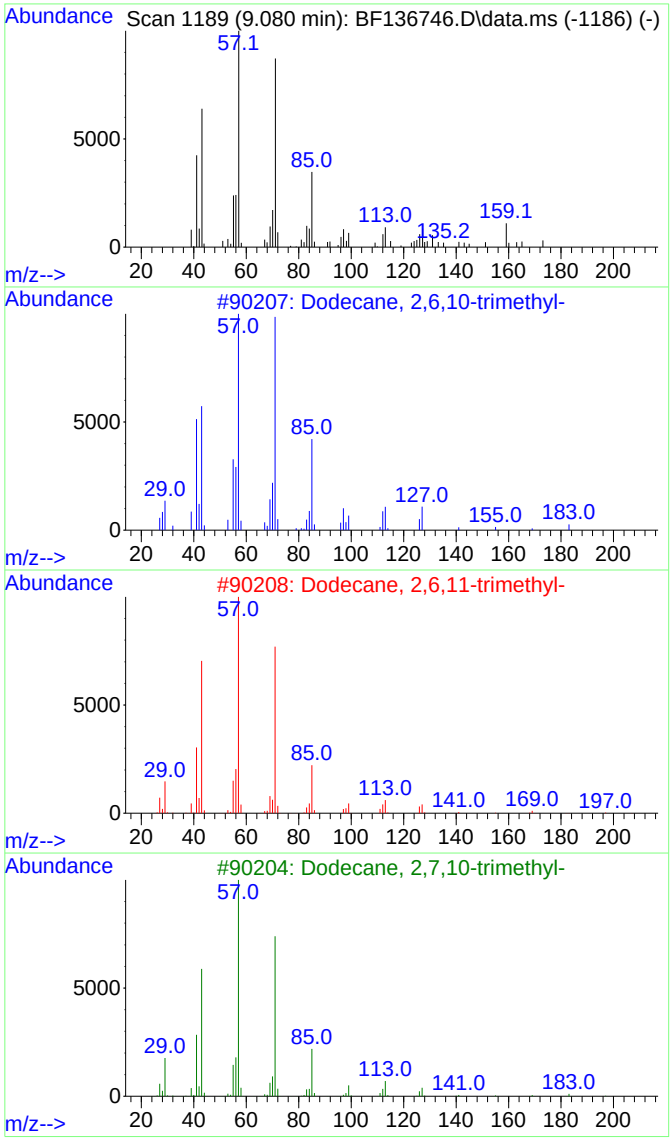
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

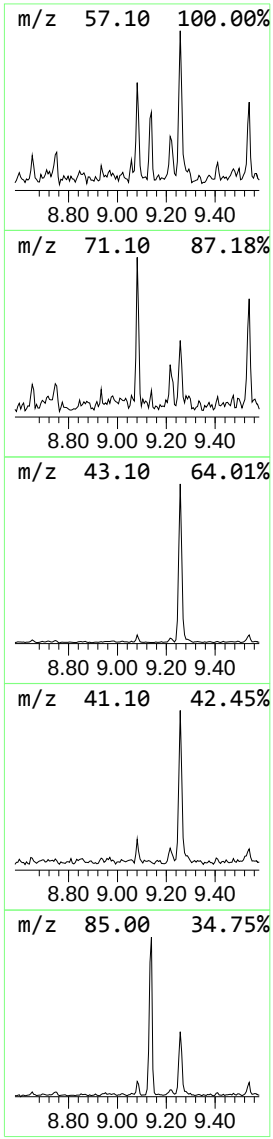
****

Peak Number 2 Dodecane, 2,6,10-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.080	2.24 ng	41067	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	90
2	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	86
3	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	78
4	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	53
5	Heptane, 3-ethyl-5-methyl-	142	C10H22	052896-90-9	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
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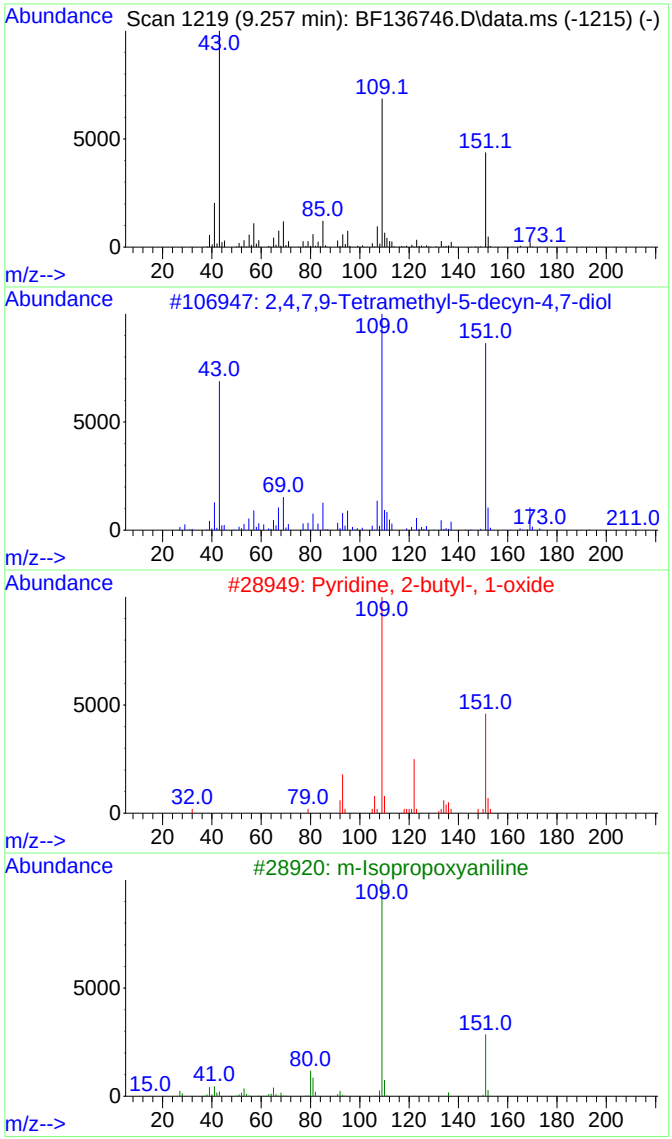
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

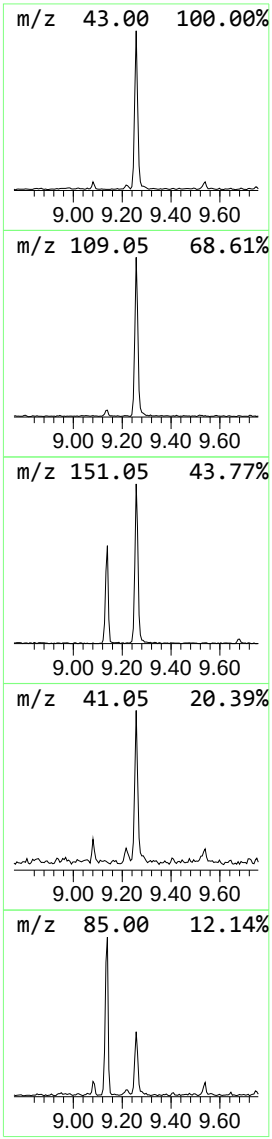
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.257	24.77 ng	453225	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	50
4	Metacetamol	151	C8H9NO2	000621-42-1	50
5	2-Thiophenecarbonitrile	109	C5H3NS	001003-31-2	38





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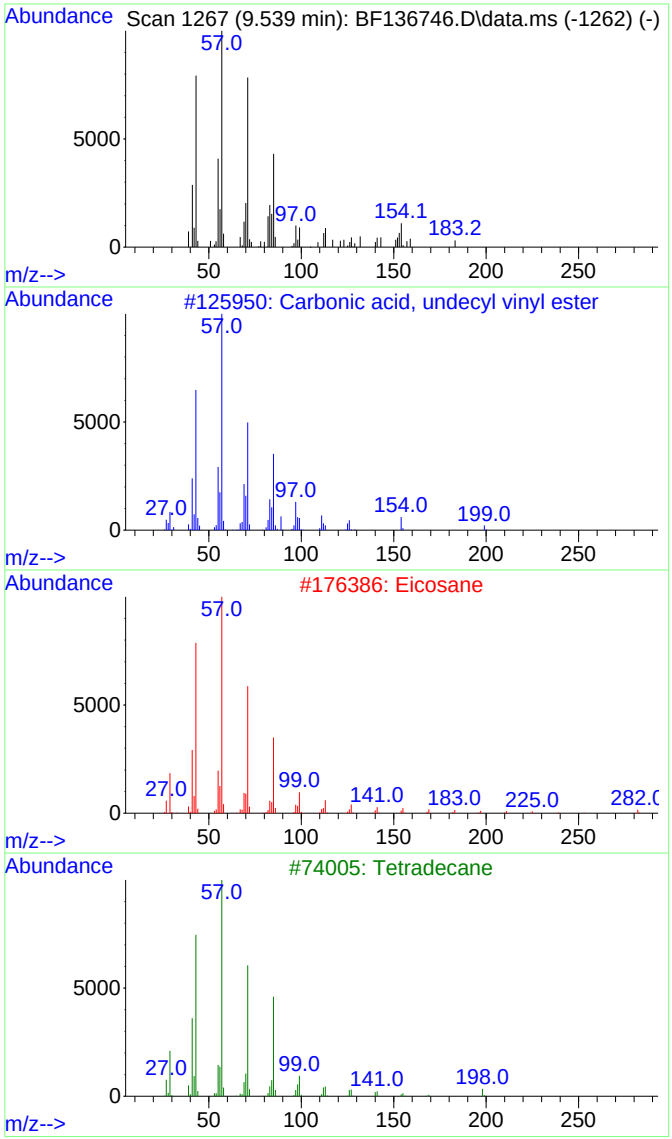
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

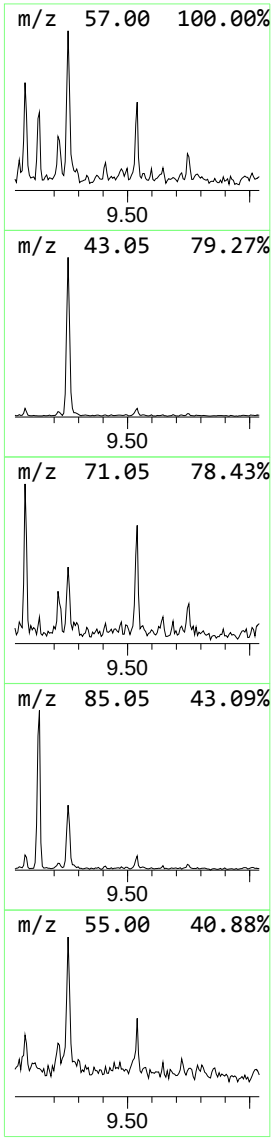
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Carbonic acid, undecyl viny... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.539	2.30 ng	41997	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, undecyl vinyl ester	242	C14H26O3	1000382-54-9	59
2	Eicosane	282	C20H42	000112-95-8	58
3	Tetradecane	198	C14H30	000629-59-4	58
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	53
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	50





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BNA_F
ClientSampleId :
NB-08-11162023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

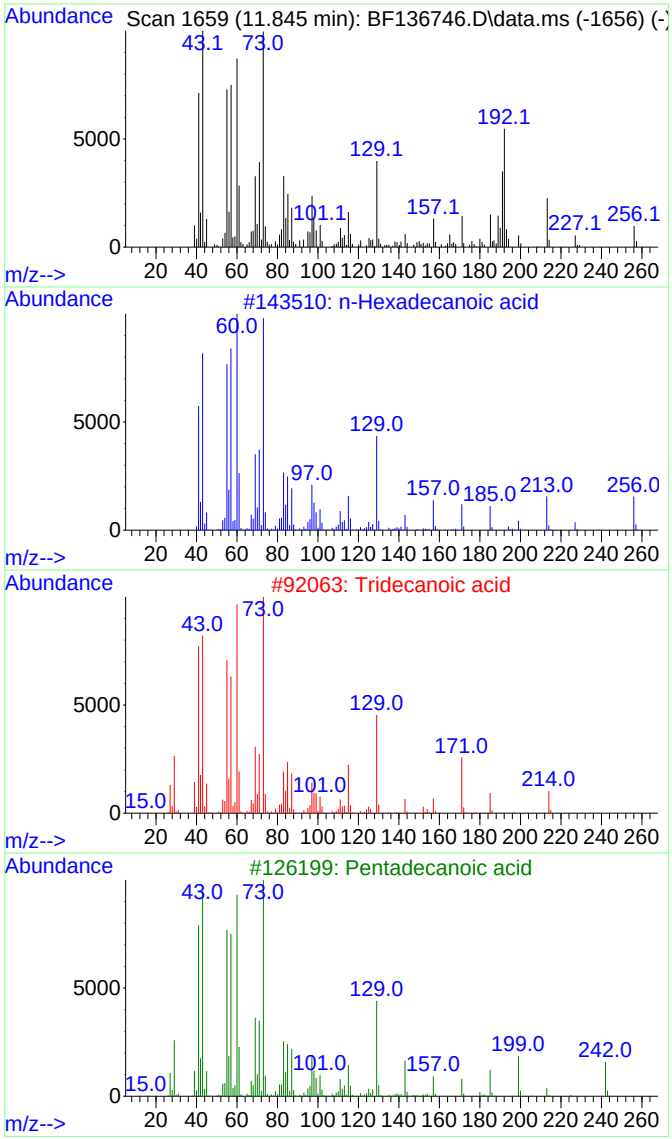
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

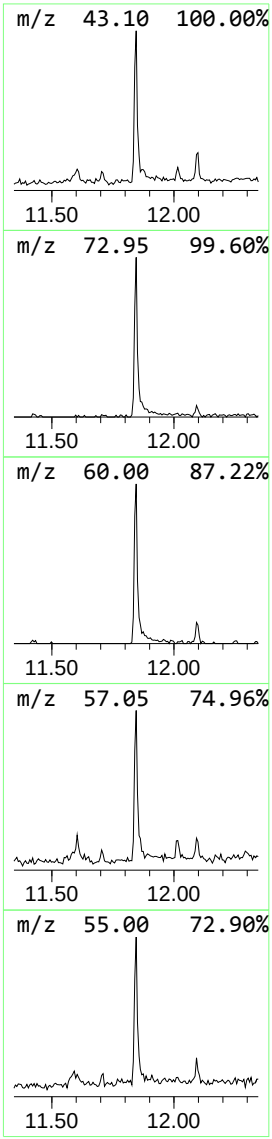
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	10.49 ng	201496	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	78
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	Octanoic acid	144	C8H16O2	000124-07-2	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
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Acq On : 27 Dec 2023 05:18
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ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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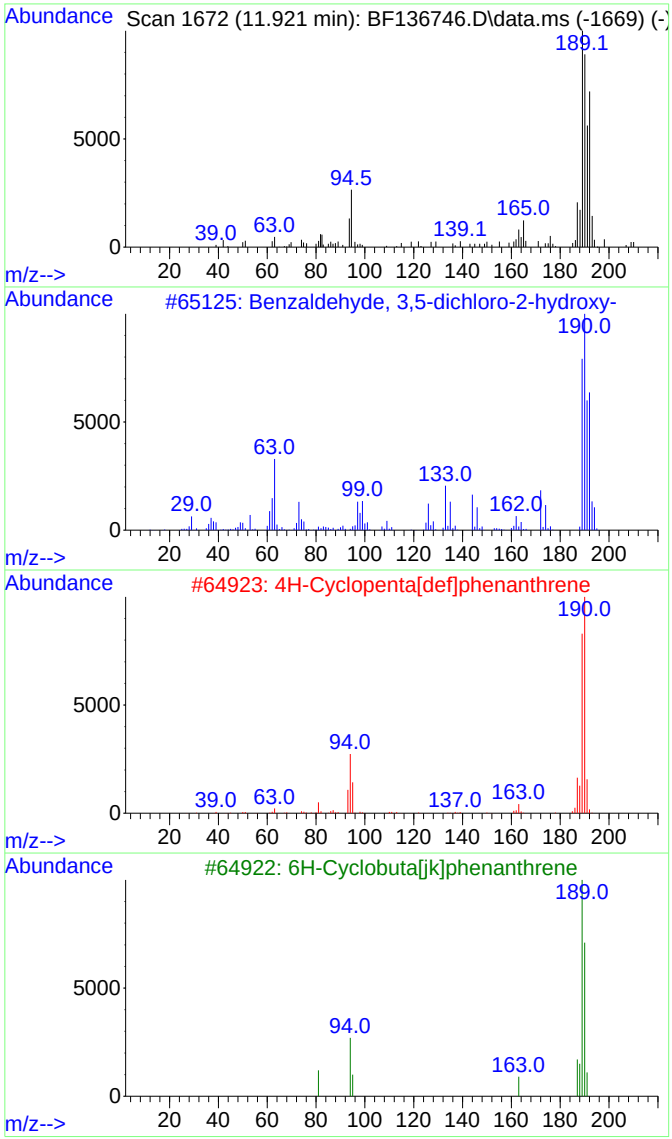
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

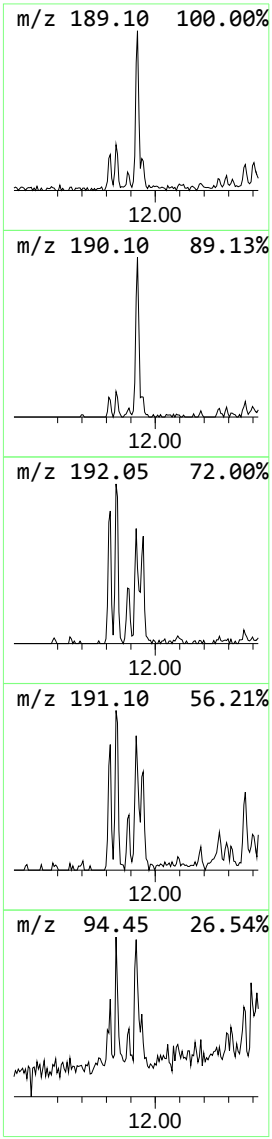
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzaldehyde, 3,5-dichloro-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	3.50 ng	67337	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	72
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	62
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	58
4	Carbonic acid, 2-formyl-4,6-dich...	276	C11H10Cl2O4	1000331-39-3	43
5	4,6-Dichloro-2-ethylpyrimidin-5-...	191	C6H7Cl2N3	006237-96-3	38





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Data File : BF136746.D
Acq On : 27 Dec 2023 05:18
Operator : CG\JU
Sample : 05463-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-11162023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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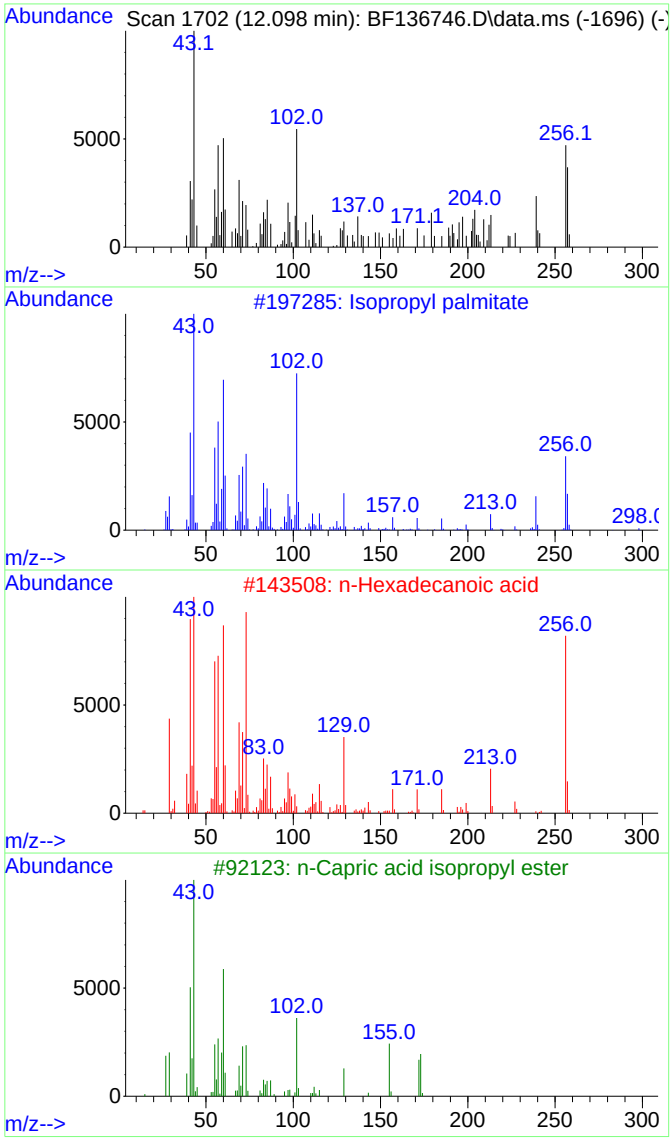
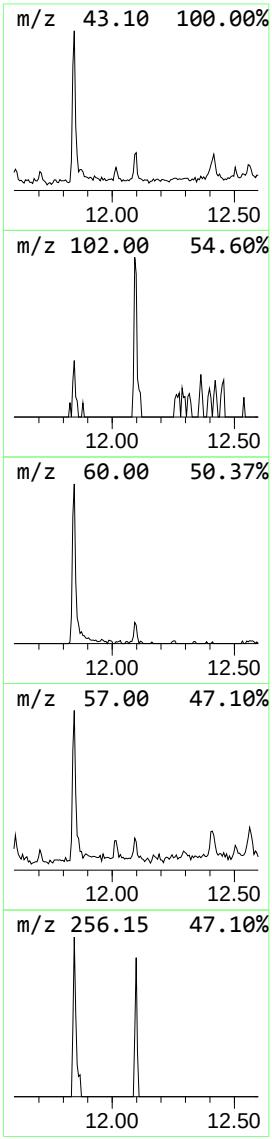
Peak Number 7 unknown12.098 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.098	3.03 ng	58183	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl palmitate	298	C19H38O2	000142-91-6	49
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	46
3	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	22
4	N-Acetyl-.alpha.-aminooxy-propio...	175	C7H13NO4	091666-51-2	22
5	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	16





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Misc :
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Instrument :
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ClientSampleId :
NB-08-11162023

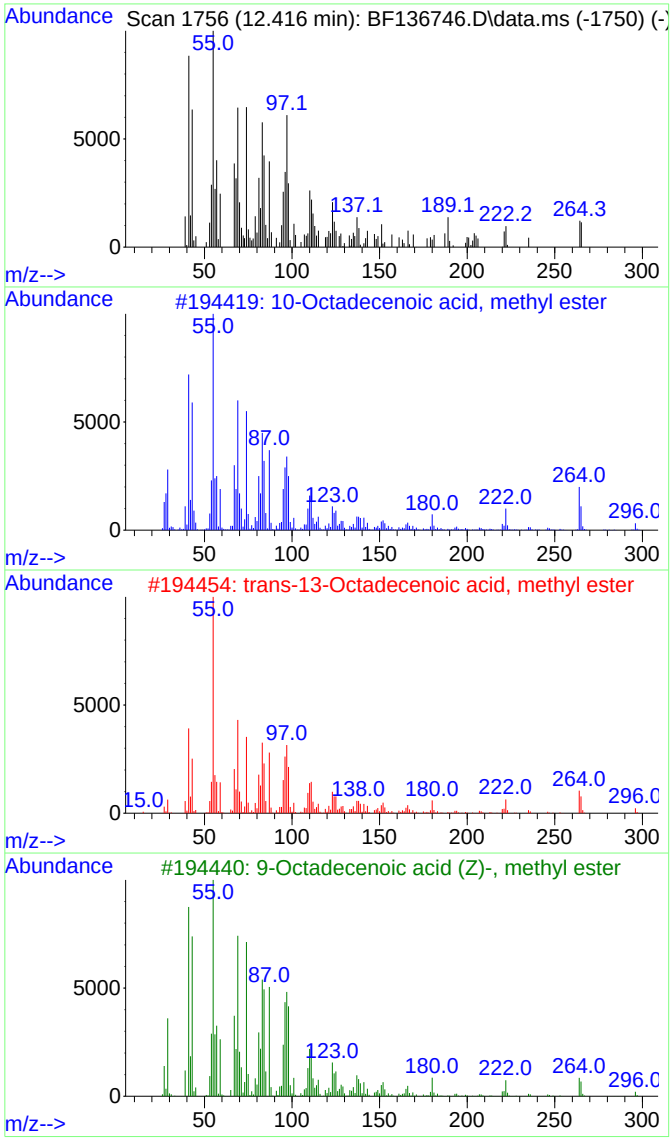
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

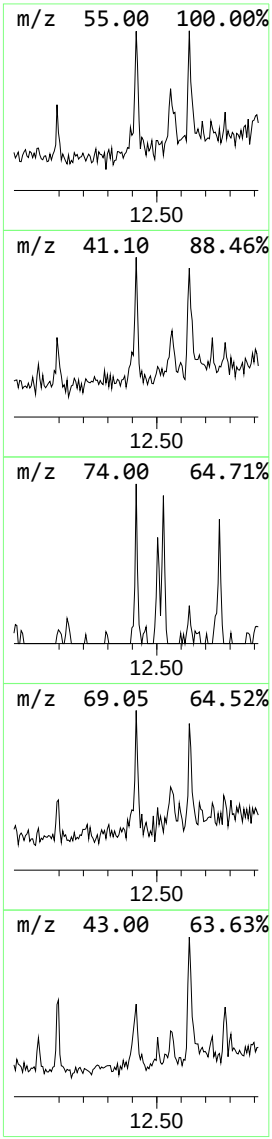
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 10-Octadecenoic acid, methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.416	5.34 ng	102621	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
2	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	90
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	68
4	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	64
5	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	62





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Sample : 05463-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

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

TIC Library : C:\Database\NIST20.L
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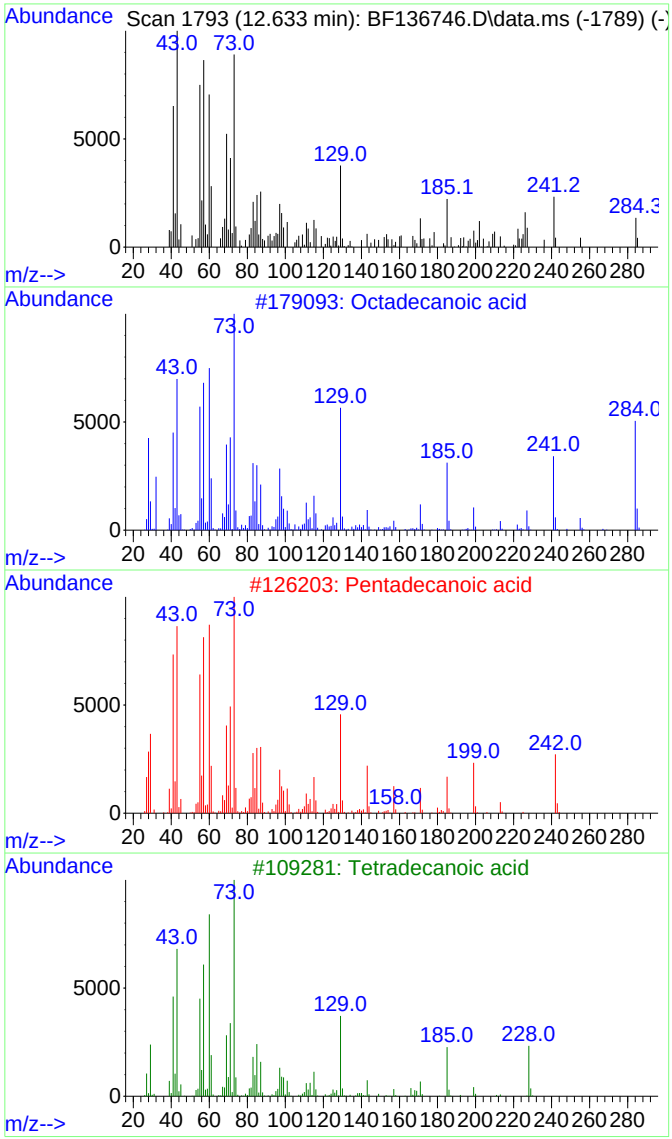
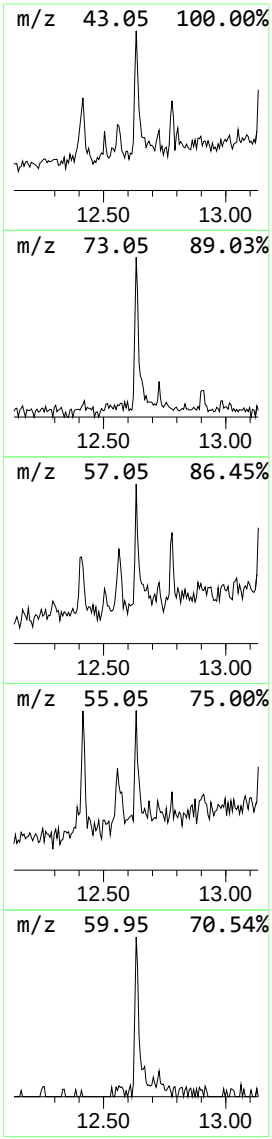
Peak Number 9 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	4.11 ng	79063	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





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TIC Library : C:\Database\NIST20.L
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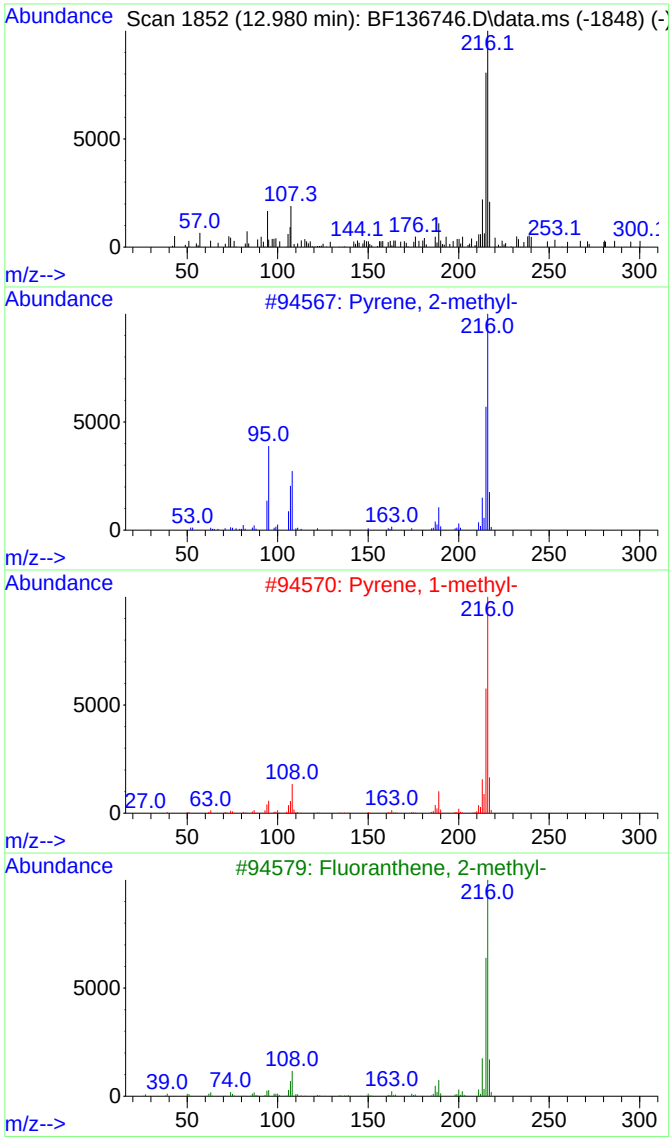
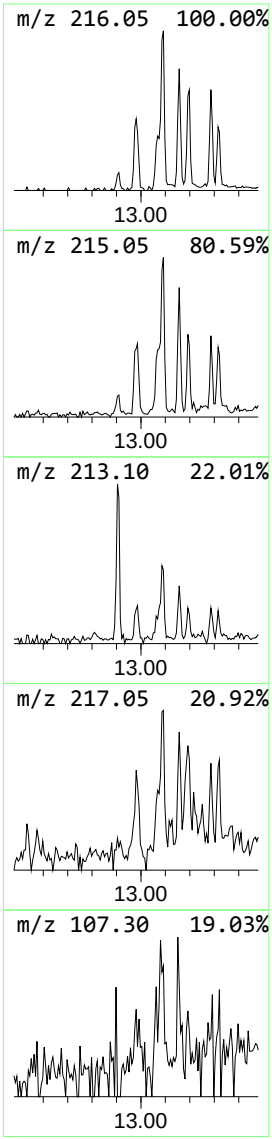
Peak Number 10 Pyrene, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.980	2.04 ng	45571	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 2-methyl-	216	C17H12	003442-78-2	93
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	76
4	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	76
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	68





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Sample : 05463-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-11162023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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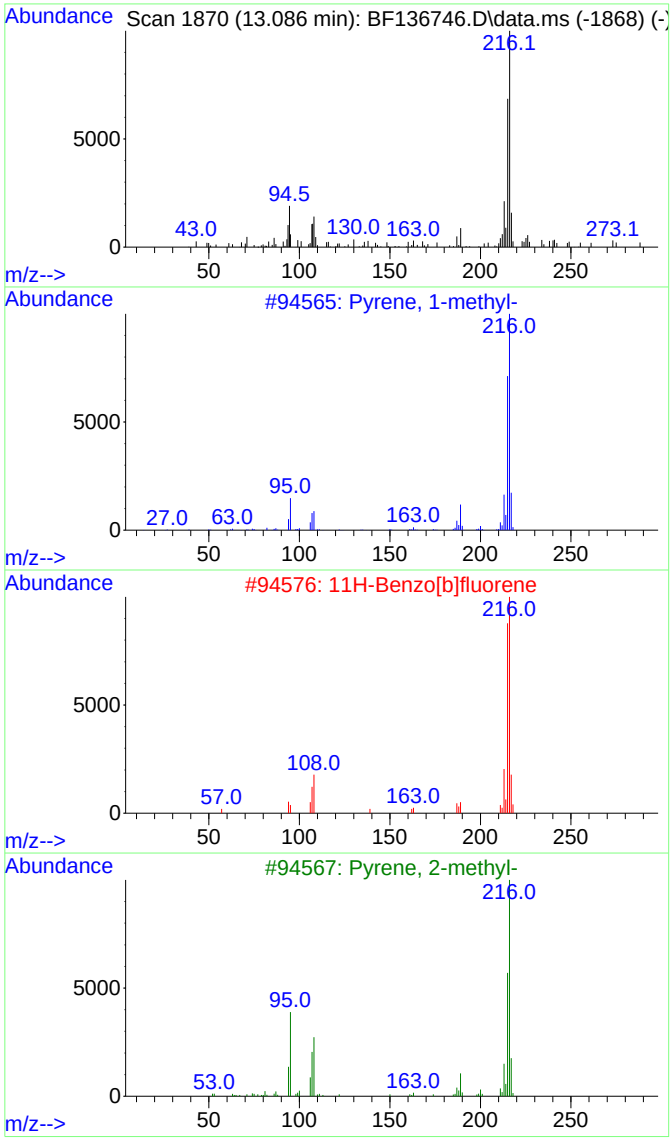
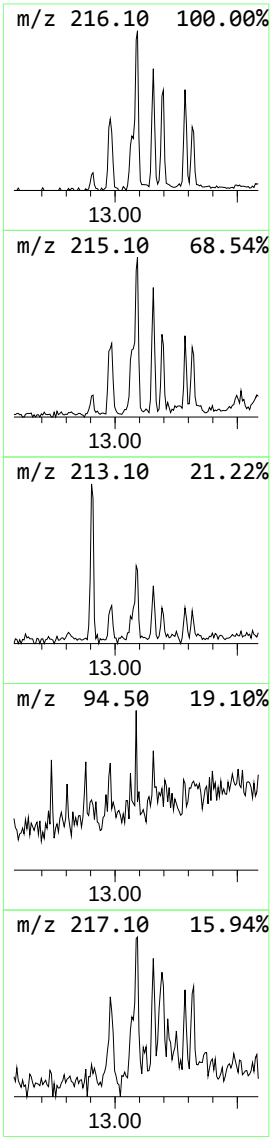
Peak Number 11 Pyrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.086	2.26 ng	50632	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	81
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	76
3	Pyrene, 2-methyl-	216	C17H12	003442-78-2	74
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	72
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	70





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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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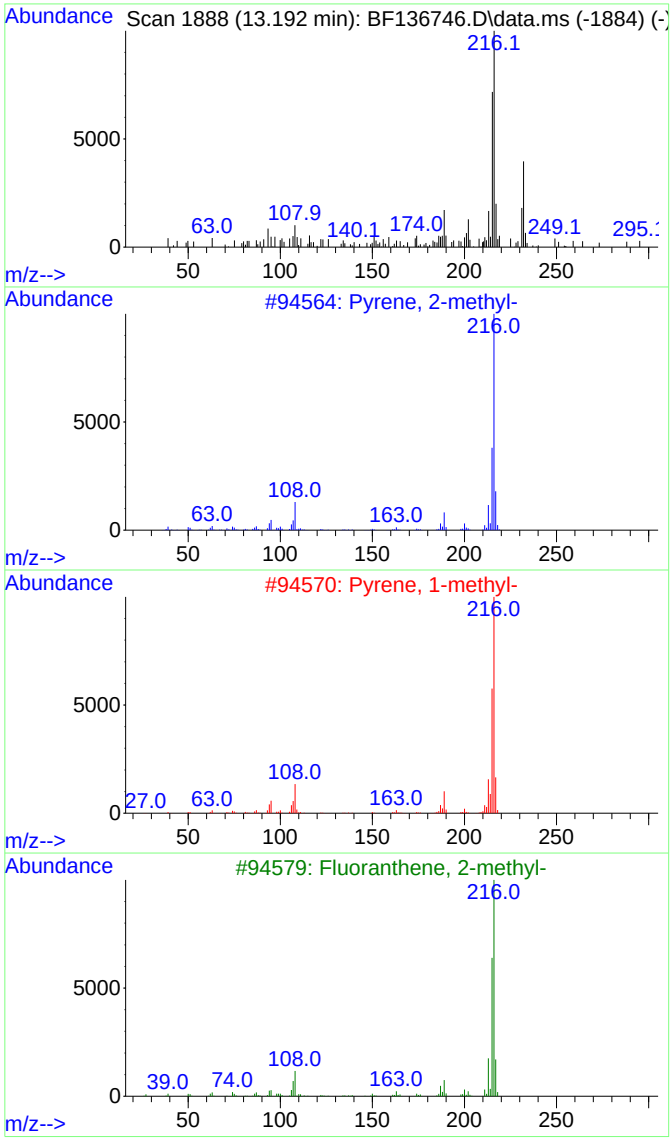
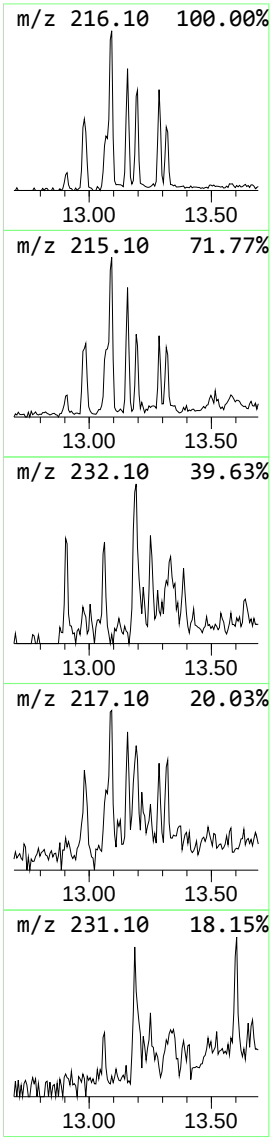
Peak Number 12 Fluoranthene, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.192	2.02 ng	45155	Chrysene-d12	13.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 2-methyl-	216	C17H12	003442-78-2	70
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	64
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	64
4	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	62
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	62





Tentatively Identified Compound (LSC) summary

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Acq On : 27 Dec 2023 05:18
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BNA_F
ClientSampleId :
NB-08-11162023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
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
2-Pentanone, 4-...	5.022	7.8	ng	132327	1	6.781	337298	20.0
Dodecane, 2,6,1...	9.080	2.2	ng	41067	3	9.816	365881	20.0
2,4,7,9-Tetrame...	9.257	24.8	ng	453225	3	9.816	365881	20.0
Carbonic acid, ...	9.539	2.3	ng	41997	3	9.816	365881	20.0
n-Hexadecanoic ...	11.845	10.5	ng	201496	4	11.310	384323	20.0
Benzaldehyde, 3...	11.922	3.5	ng	67337	4	11.310	384323	20.0
unknown12.098	12.098	3.0	ng	58183	4	11.310	384323	20.0
10-Octadecenoic...	12.416	5.3	ng	102621	4	11.310	384323	20.0
Octadecanoic acid	12.633	4.1	ng	79063	4	11.310	384323	20.0
Pyrene, 2-methyl-	12.980	2.0	ng	45571	5	13.963	447751	20.0
Pyrene, 1-methyl-	13.086	2.3	ng	50632	5	13.963	447751	20.0
Fluoranthene, 2...	13.192	2.0	ng	45155	5	13.963	447751	20.0