LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
Data File : BF135863.D
Acq On : 18 Oct 2023 23:28
Operator : CG\JU
Sample : 04887-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-622-COMP-04

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-BF101323.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135863.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.340	380	383	397	rBV	34945	71610	3.97%	0.399%
2	4.963	485	489	509	rBV	505865	719470	39.87%	4.010%
3	5.381	556	560	585	rBV	1394738	1772419	98.23%	9.878%
4	5.763	622	625	632	rBV	18798	23003	1.27%	0.128%
5	6.392	729	732	759	rBV	1703846	1769604	98.07%	9.863%
6	6.740	787	791	805	rVB	472120	450600	24.97%	2.511%
7	7.304	884	887	911	rBV	1141766	1097040	60.80%	6.114%
8	8.016	1005	1008	1010	rBV	698200	552103	30.60%	3.077%
9	8.039	1010	1012	1022	rVB	215768	208732	11.57%	1.163%
10	9.092	1188	1191	1203	rBV	2062142	1804349	100.00%	10.056%
11	9.210	1208	1211	1216	rVB	26825	26732	1.48%	0.149%
12	9.775	1303	1307	1310	rBV	770431	637323	35.32%	3.552%
13	9.804	1310	1312	1320	rVB	44295	47641	2.64%	0.266%
14	9.992	1337	1344	1348	rBV2	14886	22578	1.25%	0.126%
15	10.328	1396	1401	1407	rBV	49566	50231	2.78%	0.280%
16	10.575	1439	1443	1458	rBV	1142349	1190837	66.00%	6.637%
17	11.169	1540	1544	1549	rVB	19781	21373	1.18%	0.119%
18	11.269	1558	1561	1564	rBV	755642	711183	39.41%	3.964%
19	11.292	1564	1565	1571	rVV	468683	376234	20.85%	2.097%
20	11.351	1571	1575	1580	rVB	135125	126979	7.04%	0.708%
21	11.780	1645	1648	1650	rBV	45393	46850	2.60%	0.261%
22	11.804	1650	1652	1659	rVV3	273454	290473	16.10%	1.619%
23	11.857	1659	1661	1664	rVV	35405	38280	2.12%	0.213%
24	11.892	1664	1667	1669	rVV	104832	107236	5.94%	0.598%
25	11.916	1669	1671	1676	rVB2	32512	31786	1.76%	0.177%
26	12.051	1690	1694	1696	rBV2	27203	23064	1.28%	0.129%
27	12.074	1696	1698	1703	rVB	41682	37395	2.07%	0.208%
28	12.127	1703	1707	1710	rBV	16551	19992	1.11%	0.111%
29	12.333	1737	1742	1744	rBV	23336	26698	1.48%	0.149%
30	12.369	1744	1748	1751	rVV5	15286	23716	1.31%	0.132%
31	12.433	1757	1759	1766	rVB	20934	25950	1.44%	0.145%
32	12.492	1766	1769	1776	rBV	640597	625574	34.67%	3.487%
33	12.598	1784	1787	1793	rBV5	25607	40549	2.25%	0.226%
34	12.651	1793	1796	1802	rVV	29791	33589	1.86%	0.187%
35	12.727	1802	1809	1815	rVV	488918	570356	31.61%	3.179%
36	12.780	1815	1818	1822	rVB	19831	20905	1.16%	0.117%

LSC Area Percent Report

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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

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Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.869	1828	1833	1836	rBV	1552932	1510221	83.70%	8.417%
38	12.945	1842	1846	1847	rBV	23825	27771	1.54%	0.155%
39	13.063	1863	1866	1869	rVB	56490	53663	2.97%	0.299%
40	13.127	1874	1877	1880	rVV	50832	43862	2.43%	0.244%
41	13.163	1880	1883	1890	rVB3	32261	46647	2.59%	0.260%
42	13.592	1953	1956	1969	rVB3	14539	31202	1.73%	0.174%
43	13.686	1969	1972	1974	rBV	25726	29587	1.64%	0.165%
44	13.710	1974	1976	1979	rVB	28414	24344	1.35%	0.136%
45	13.739	1979	1981	1983	rBV	24168	22932	1.27%	0.128%
46	13.768	1983	1986	1989	rVV2	24673	29328	1.63%	0.163%
47	13.804	1989	1992	1994	rVV	22129	23545	1.30%	0.131%
48	13.857	1996	2001	2007	rVV5	37752	93413	5.18%	0.521%
49	13.933	2010	2014	2017	rVV2	466645	615529	34.11%	3.431%
50	13.963	2017	2019	2026	rVV	173806	193809	10.74%	1.080%
51	14.027	2026	2030	2031	rVV	39155	43140	2.39%	0.240%
52	14.045	2031	2033	2038	rVB	49827	46506	2.58%	0.259%
53	14.333	2077	2082	2086	rBV2	32249	39224	2.17%	0.219%
54	14.398	2090	2093	2096	rVV3	17345	20664	1.15%	0.115%
55	14.686	2138	2142	2147	rBV3	43650	61016	3.38%	0.340%
56	14.768	2153	2156	2159	rVB	43560	43981	2.44%	0.245%
57	14.845	2165	2169	2174	rBV4	17857	30711	1.70%	0.171%
58	14.986	2189	2193	2196	rBV	153032	208424	11.55%	1.162%
59	15.104	2209	2213	2217	rBV	29493	39391	2.18%	0.220%
60	15.292	2241	2245	2249	rVB	89763	97946	5.43%	0.546%
61	15.357	2252	2256	2261	rVB	132721	153084	8.48%	0.853%
62	15.415	2261	2266	2270	rBV	382672	495600	27.47%	2.762%
63	15.845	2336	2339	2343	rVB2	17595	22047	1.22%	0.123%
64	15.992	2361	2364	2369	rVB4	12965	20342	1.13%	0.113%
65	16.933	2518	2524	2531	rBV	64312	132703	7.35%	0.740%
66	17.392	2596	2602	2610	rBV	40418	99594	5.52%	0.555%

Sum of corrected areas: 17942680

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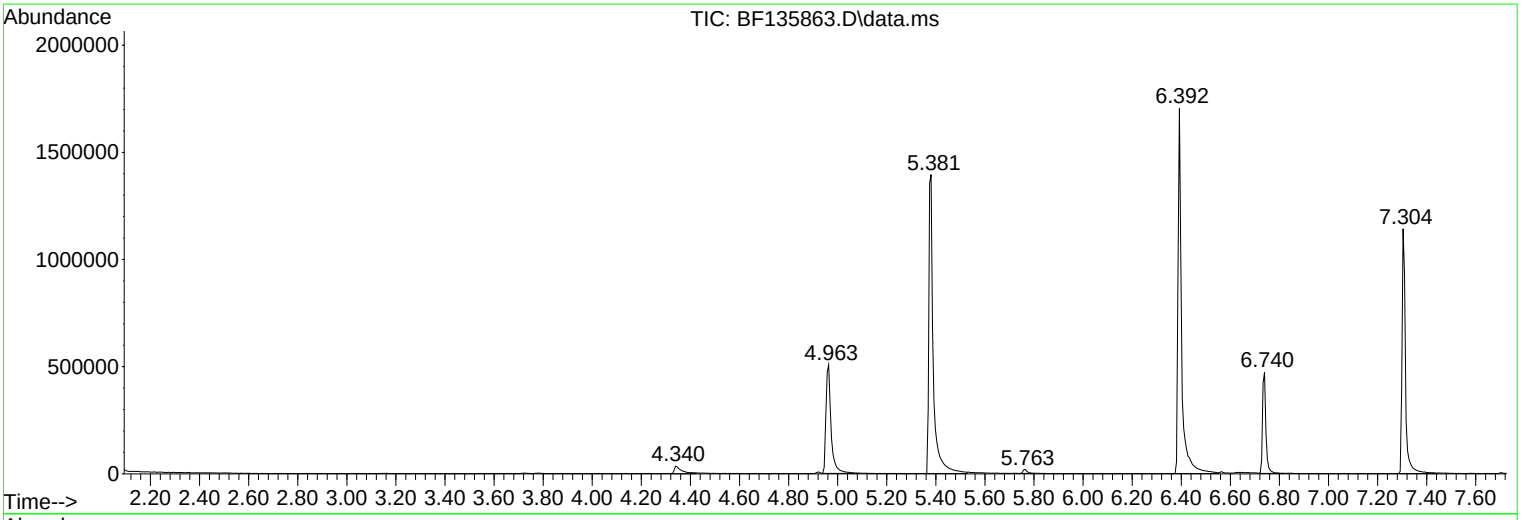
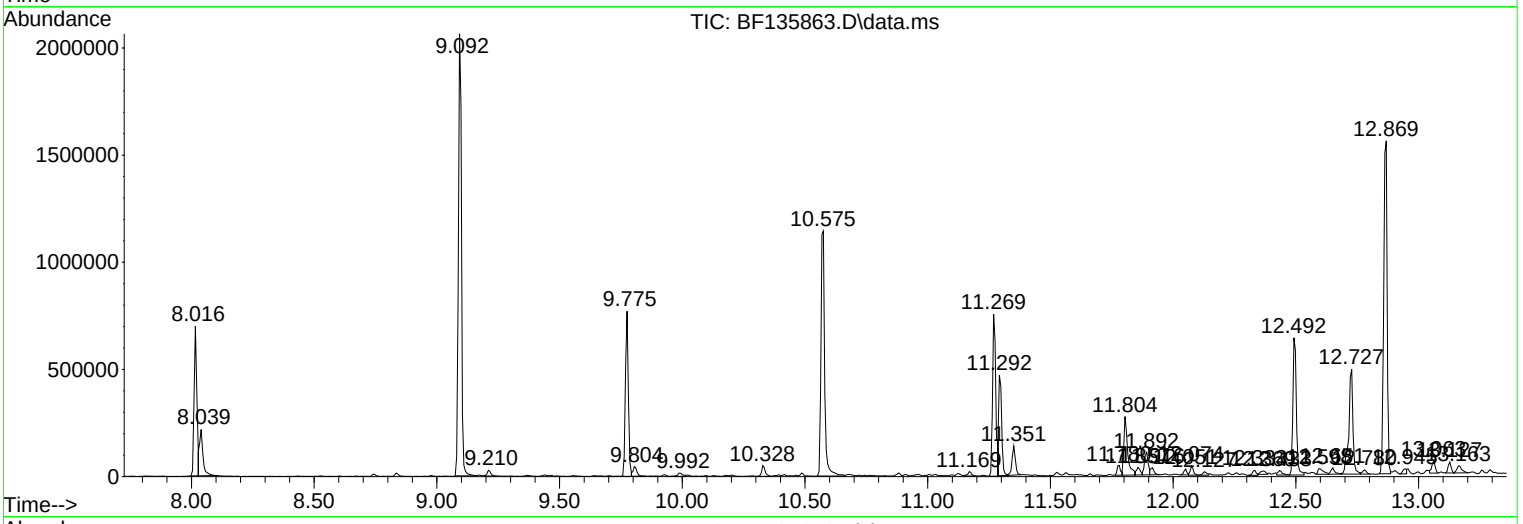
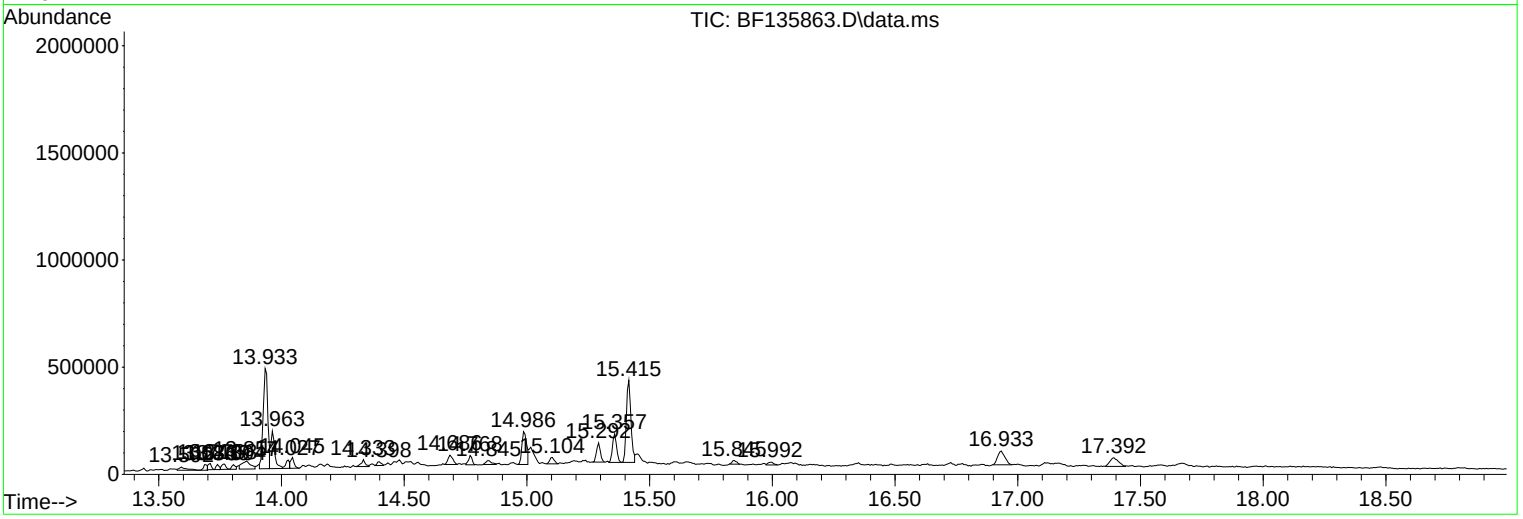
ClientSampleId :
SU-622-COMP-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

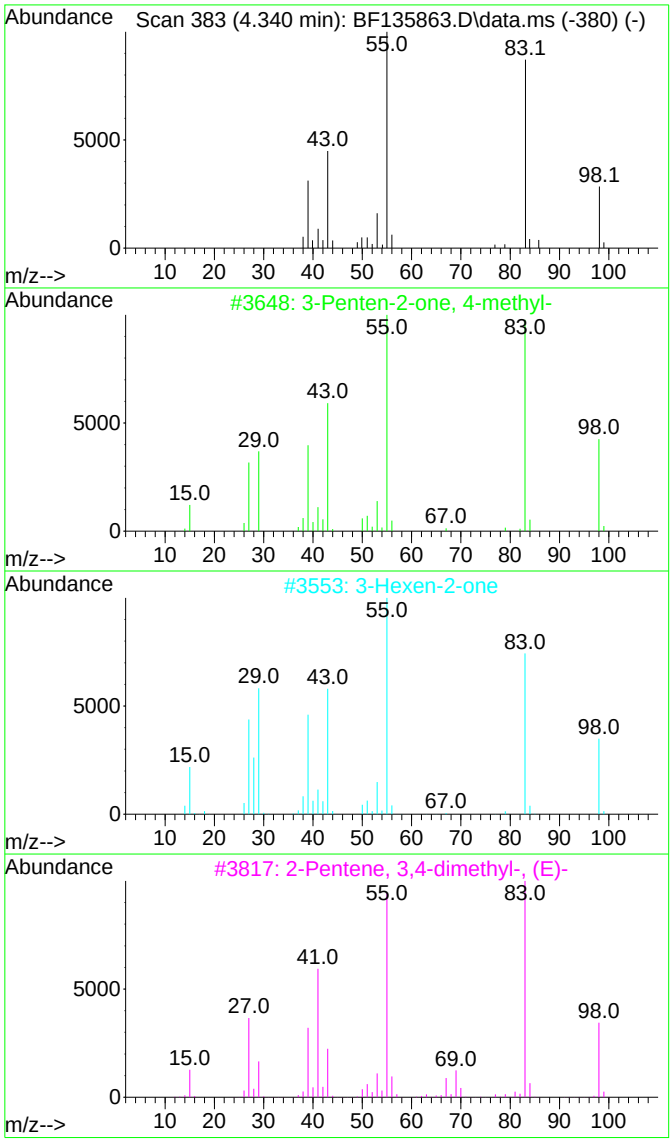
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

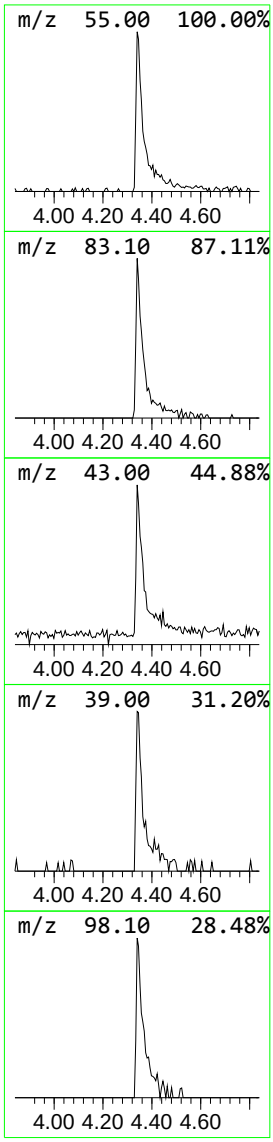
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.340	3.18 ng	71610	1,4-Dichlorobenzene-d4	6.740

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
5	Furan, 2,5-dihydro-2,5-dimethyl-	98	C6H10O	059242-27-2	72





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

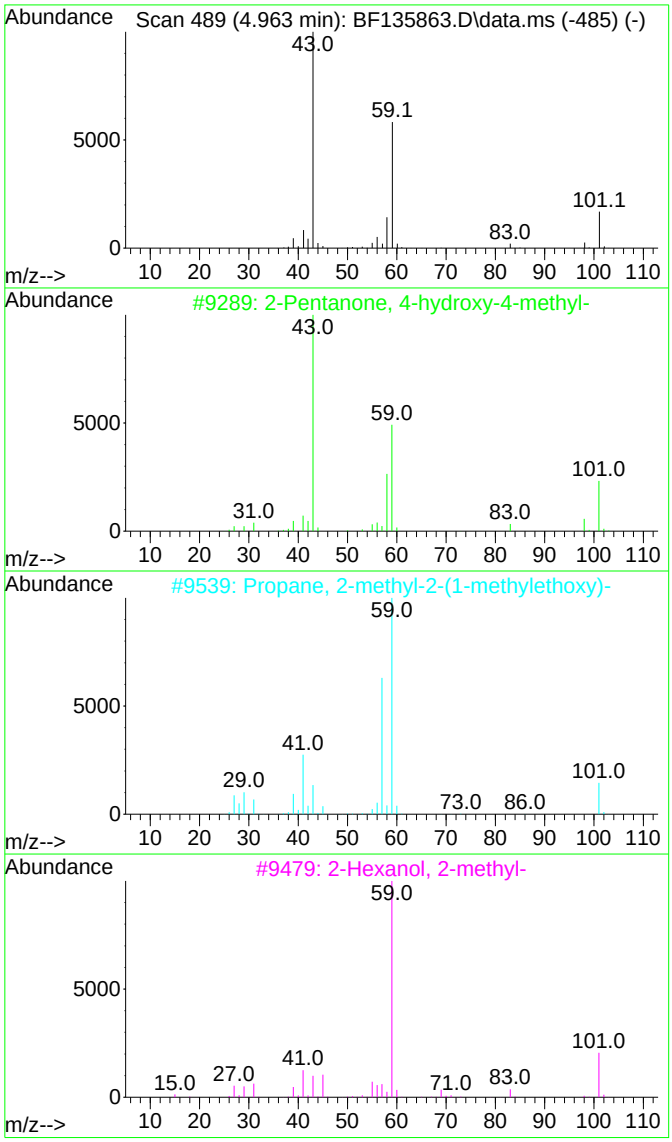
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

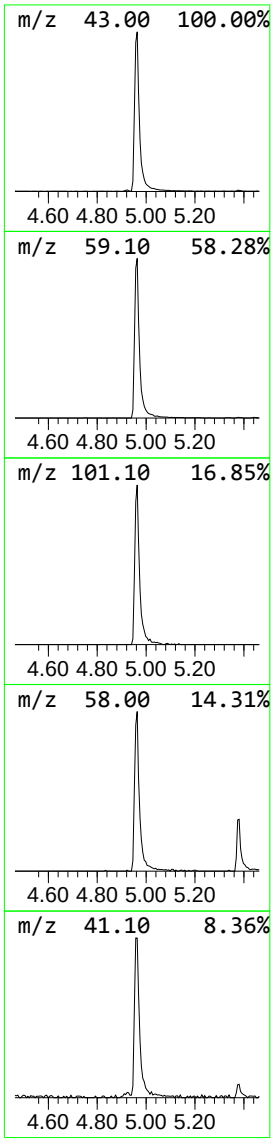
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	31.93 ng	719470	1,4-Dichlorobenzene-d4	6.740

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
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Sample : 04887-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-622-COMP-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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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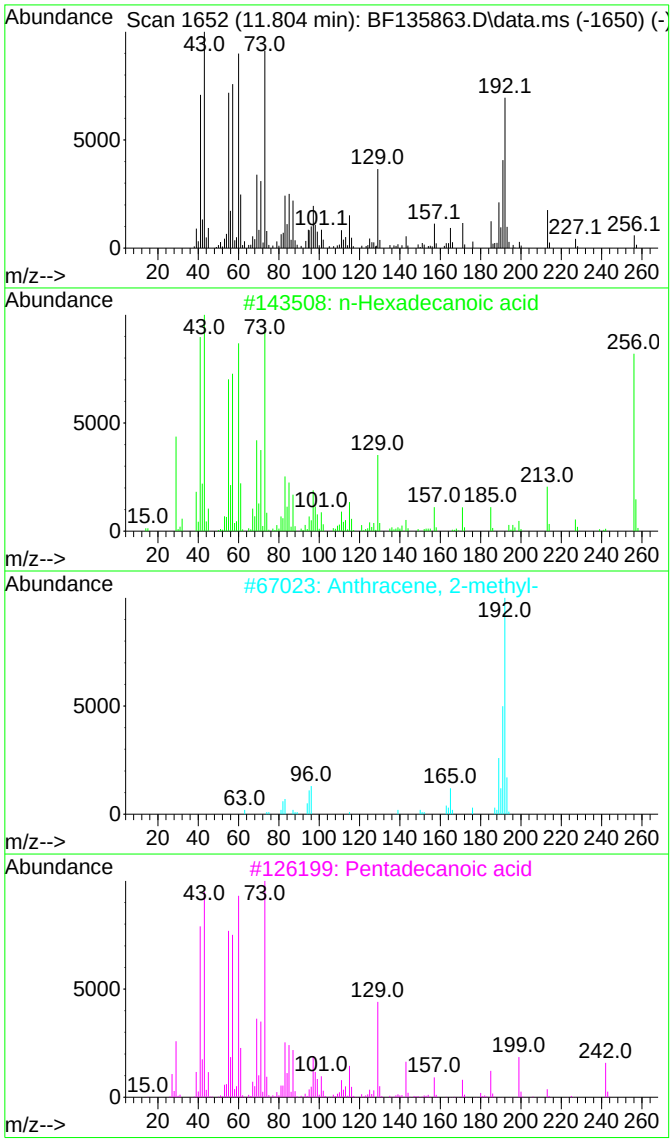
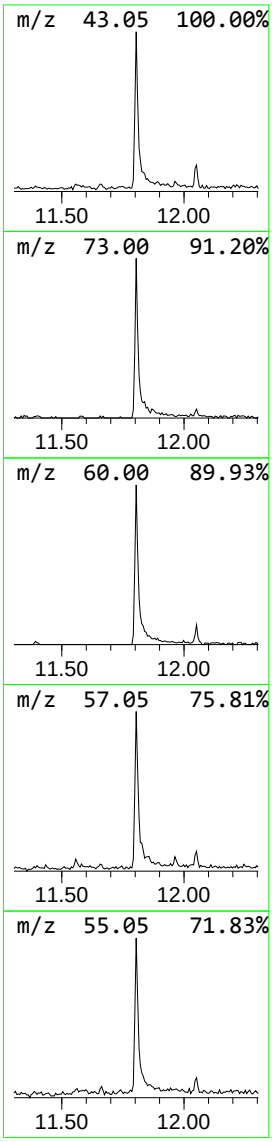
Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	8.17 ng	290473	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	78
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	56





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TIC Library : C:\Database\NIST20.L
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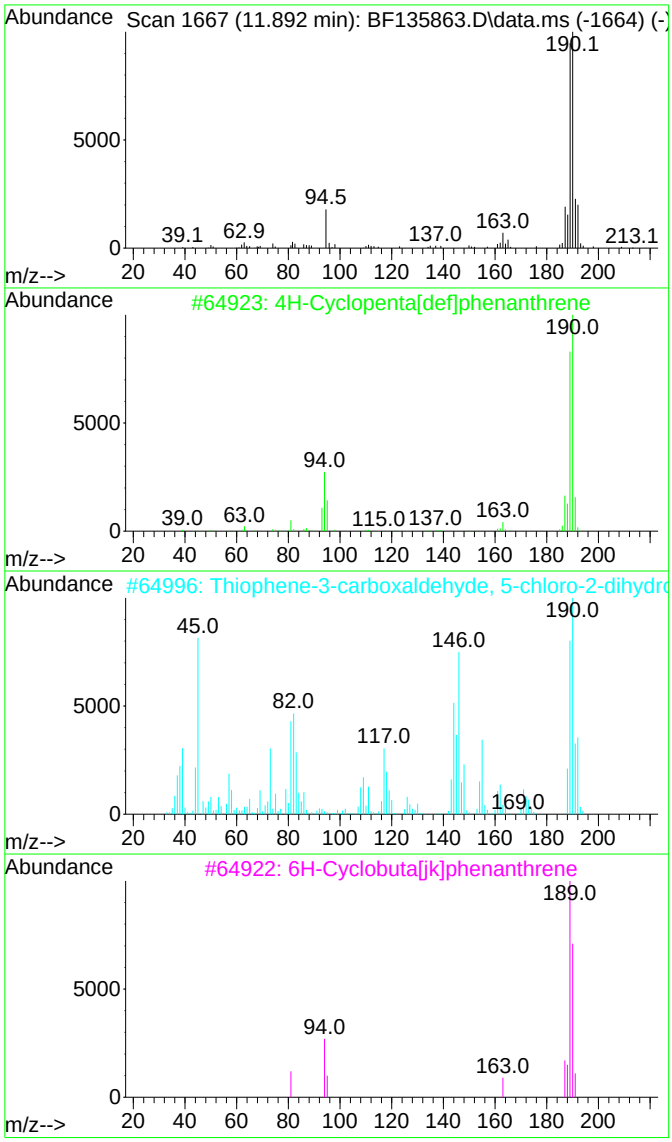
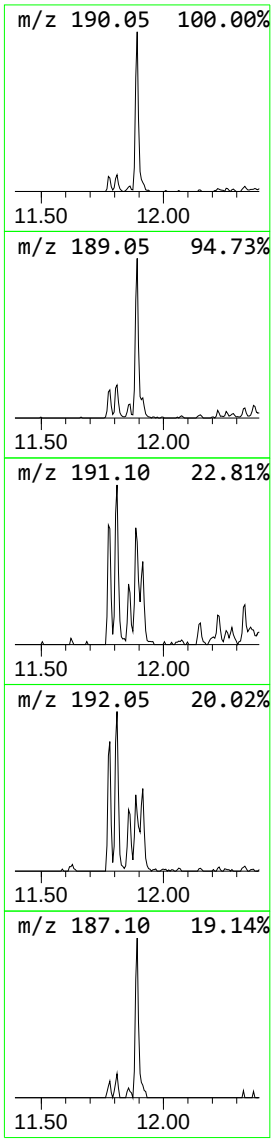
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	3.02 ng	107236	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	59
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
4	Methyl diselenide	190	C2H6Se2	007101-31-7	49
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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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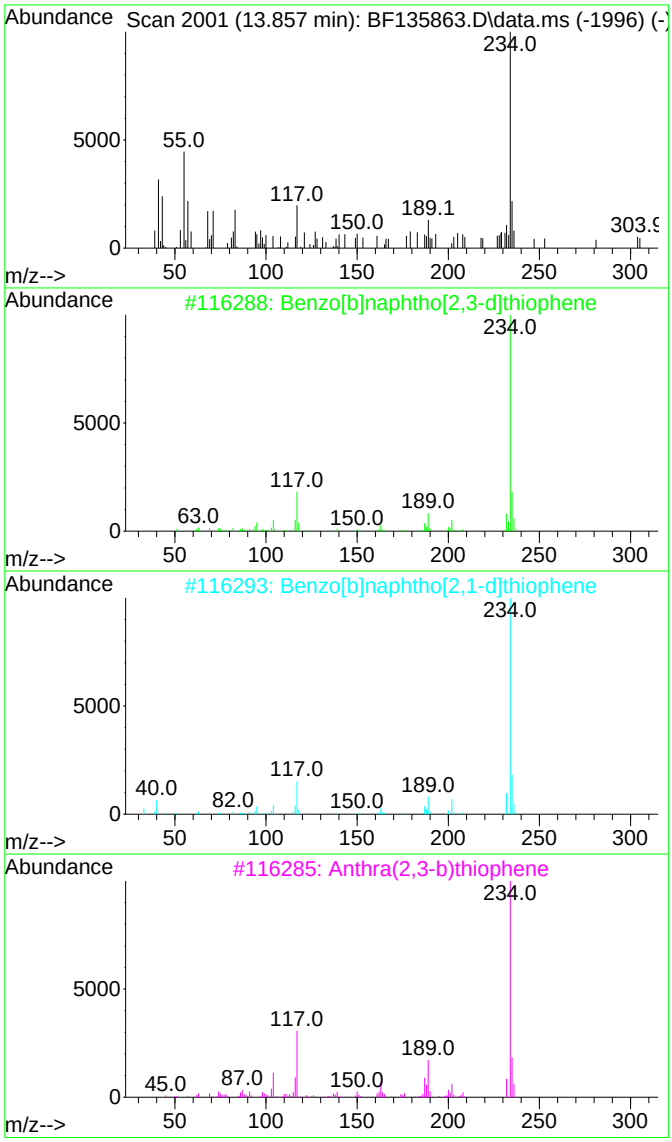
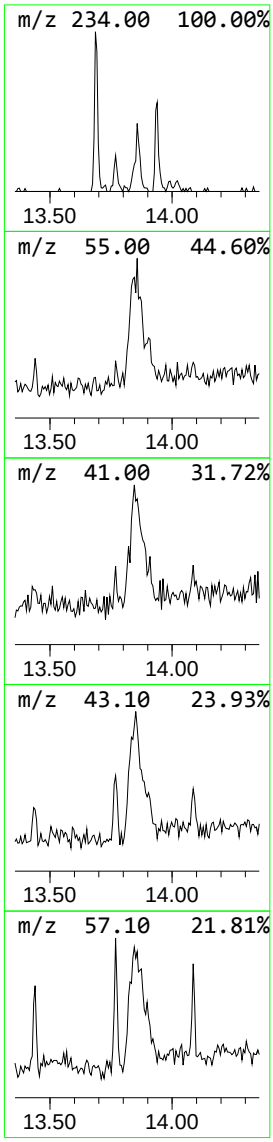
Peak Number 5 Benzo[b]naphtho[2,3-d]thiop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	3.04 ng	93413	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]naphtho[2,3-d]thiophene	234	C16H10S	000243-46-9	91
2	Benzo[b]naphtho[2,1-d]thiophene	234	C16H10S	000239-35-0	87
3	Anthra(2,3-b)thiophene	234	C16H10S	022108-55-0	83
4	Imidazole, 4-pentafluorophenyl-	234	C9H3F5N2	081769-58-6	64
5	Phenanthro[4,3-b]thiophene	234	C16H10S	000195-68-6	64





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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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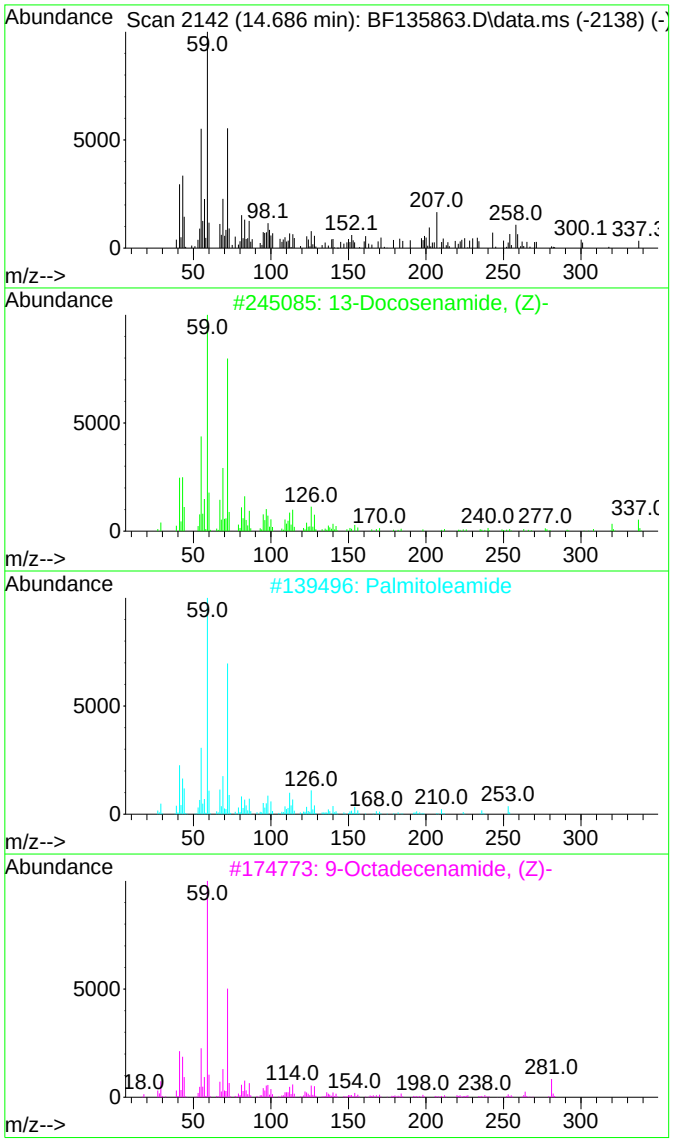
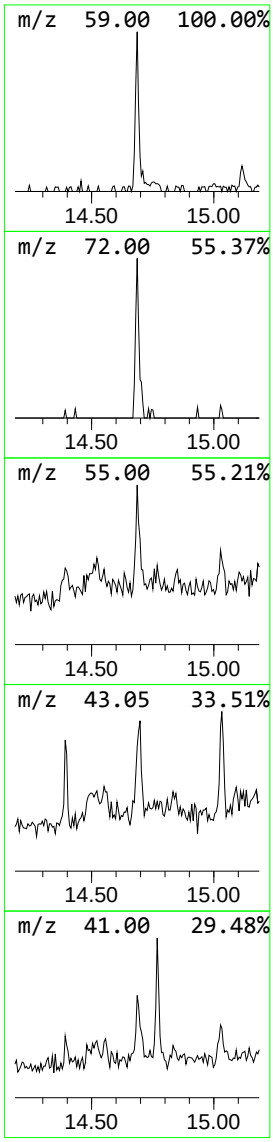
Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.686	2.46 ng	61016	Perylene-d12	15.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	95
2	Palmitoleamide	253	C16H31NO	106010-22-4	92
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
4	Decanamide-	171	C10H21NO	002319-29-1	46
5	Octanamide	143	C8H17NO	000629-01-6	43





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Data File : BF135863.D
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Operator : CG\JU
Sample : 04887-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-622-COMP-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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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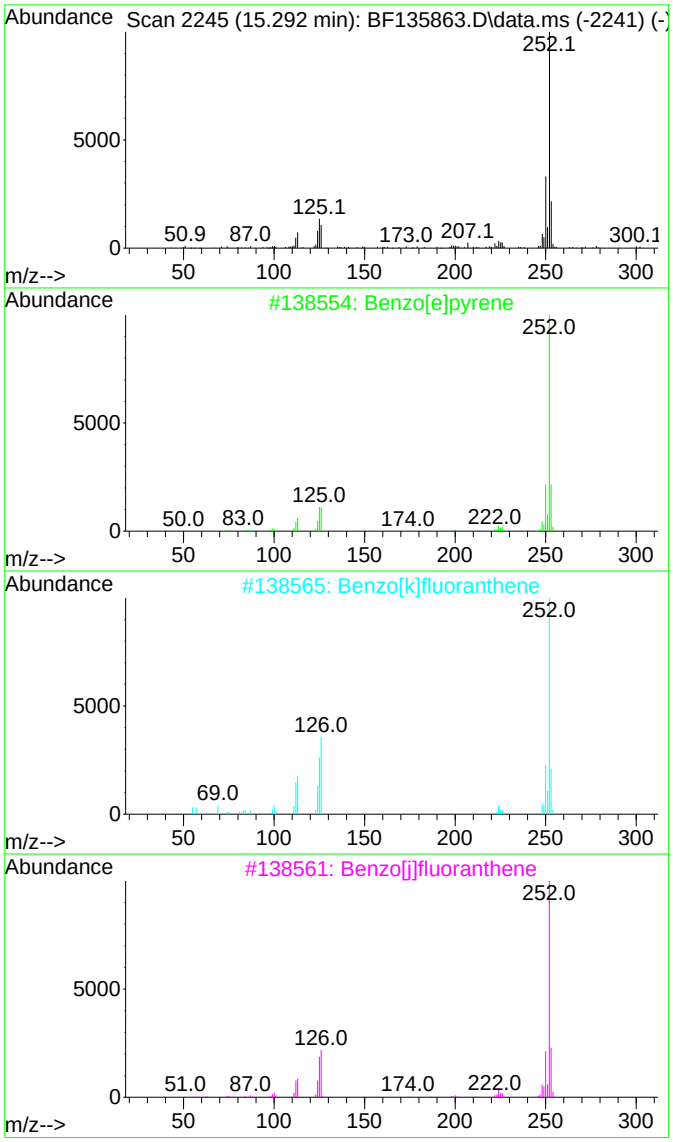
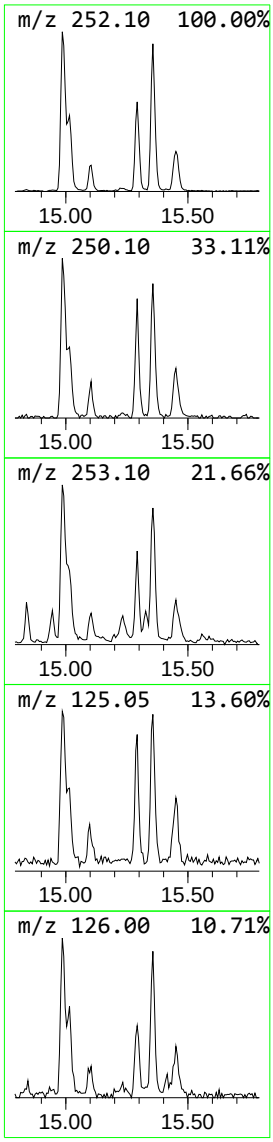
Peak Number 7 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.292	3.95 ng	97946	Perylene-d12	15.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
5	Benzo[a]pyrene	252	C20H12	000050-32-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
Data File : BF135863.D
Acq On : 18 Oct 2023 23:28
Operator : CG\JU
Sample : 04887-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-622-COMP-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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
3-Penten-2-one,...	4.340	3.2	ng	71610	1	6.740	450600	20.0
2-Pentanone, 4-...	4.963	31.9	ng	719470	1	6.740	450600	20.0
n-Hexadecanoic ...	11.804	8.2	ng	290473	4	11.269	711183	20.0
4H-Cyclopenta[d...	11.892	3.0	ng	107236	4	11.269	711183	20.0
Benzo[b]naphtho...	13.857	3.0	ng	93413	5	13.939	615529	20.0
13-Docosenamide...	14.686	2.5	ng	61016	6	15.415	495600	20.0
Benzo[e]pyrene	15.292	4.0	ng	97946	6	15.415	495600	20.0