LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133044.D
Acq On : 26 Apr 2023 00:02
Operator : CG\JU
Sample : 02270-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-19-0-2-20230411

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133044.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	12	rVB2	51893	57127	1.08%	0.121%
2	4.299	372	376	383	rVB	108318	124493	2.36%	0.263%
3	4.940	479	485	495	rVB	1254689	1653497	31.34%	3.495%
4	5.357	551	556	559	rBV	4513591	4726489	89.58%	9.991%
5	5.751	619	623	626	rBV	103193	95367	1.81%	0.202%
6	6.381	724	730	733	rBV	4549439	4834156	91.62%	10.219%
7	6.740	787	791	794	rBV	1456038	1143347	21.67%	2.417%
8	7.304	881	887	890	rBV	3490792	3112199	58.99%	6.579%
9	8.022	1005	1009	1012	rBV	1931714	1547535	29.33%	3.271%
10	9.098	1187	1192	1196	rBV	5501949	5276106	100.00%	11.153%
11	9.775	1303	1307	1310	rBV	2151282	1697551	32.17%	3.588%
12	9.804	1310	1312	1315	rVB	123141	90737	1.72%	0.192%
13	9.975	1338	1341	1344	rBV	69432	56346	1.07%	0.119%
14	10.316	1396	1399	1402	rBV	91920	77282	1.46%	0.163%
15	10.486	1424	1428	1432	rVB2	193156	165056	3.13%	0.349%
16	10.563	1436	1441	1444	rBV	3449857	3152868	59.76%	6.665%
17	10.686	1459	1462	1468	rVB4	56236	73066	1.38%	0.154%
18	11.257	1555	1559	1561	rBV	1881384	1753076	33.23%	3.706%
19	11.275	1561	1562	1566	rVV	893232	680336	12.89%	1.438%
20	11.328	1568	1571	1574	rVB	230762	184197	3.49%	0.389%
21	11.480	1592	1597	1600	rBV2	104376	101385	1.92%	0.214%
22	11.757	1640	1644	1646	rBV	111391	97489	1.85%	0.206%
23	11.792	1646	1650	1654	rVV2	345991	415599	7.88%	0.879%
24	11.827	1654	1656	1659	rVV2	74817	75492	1.43%	0.160%
25	11.869	1659	1663	1665	rVV	181183	200288	3.80%	0.423%
26	11.886	1665	1666	1671	rVB	78888	60605	1.15%	0.128%
27	12.051	1691	1694	1696	rBV	83766	79069	1.50%	0.167%
28	12.304	1734	1737	1741	rBV	66858	75979	1.44%	0.161%
29	12.386	1749	1751	1757	rVB3	61282	68671	1.30%	0.145%
30	12.463	1761	1764	1768	rBV	1422906	1228452	23.28%	2.597%
31	12.516	1768	1773	1778	rBV5	36011	72020	1.37%	0.152%
32	12.580	1781	1784	1788	rBV2	65720	86867	1.65%	0.184%
33	12.692	1797	1803	1806	rBV	1285389	1267101	24.02%	2.678%
34	12.739	1808	1811	1817	rVB3	48498	84005	1.59%	0.178%
35	12.810	1821	1823	1825	rBV	67842	58710	1.11%	0.124%
36	12.845	1825	1829	1832	rVV	5330148	4781873	90.63%	10.108%

LSC Area Percent Report

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Misc :
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Instrument :
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ClientSampleId :
SB-19-0-2-20230411

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

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Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.916	1836	1841	1843	rBV2	75756	104281	1.98%	0.220%
38	13.022	1856	1859	1862	rVB	176327	168508	3.19%	0.356%
39	13.086	1867	1870	1873	rBV	160891	138230	2.62%	0.292%
40	13.122	1873	1876	1879	rBV	122130	131418	2.49%	0.278%
41	13.216	1889	1892	1895	rBV	70073	64383	1.22%	0.136%
42	13.245	1895	1897	1900	rBV2	66586	59110	1.12%	0.125%
43	13.521	1942	1944	1951	rVB	90319	88551	1.68%	0.187%
44	13.639	1960	1964	1967	rBV2	118872	148000	2.81%	0.313%
45	13.669	1967	1969	1971	rVV	89932	79401	1.50%	0.168%
46	13.686	1971	1972	1977	rVV3	66247	90354	1.71%	0.191%
47	13.733	1977	1980	1982	rVB2	70892	69634	1.32%	0.147%
48	13.886	2002	2006	2009	rBV2	1485012	1864110	35.33%	3.940%
49	13.916	2009	2011	2017	rVB	542450	482421	9.14%	1.020%
50	13.992	2022	2024	2027	rVB	127643	104522	1.98%	0.221%
51	14.074	2035	2038	2040	rBV2	79354	69249	1.31%	0.146%
52	14.098	2040	2042	2048	rVB2	64721	102249	1.94%	0.216%
53	14.274	2070	2072	2075	rVB	88104	76309	1.45%	0.161%
54	14.374	2086	2089	2091	rBV4	60690	84899	1.61%	0.179%
55	14.816	2161	2164	2168	rVB3	106374	105390	2.00%	0.223%
56	14.904	2175	2179	2182	rBV	580226	815908	15.46%	1.725%
57	15.004	2193	2196	2200	rVB2	177387	200309	3.80%	0.423%
58	15.192	2224	2228	2234	rVB	364715	449236	8.51%	0.950%
59	15.251	2234	2238	2244	rVB	466809	507628	9.62%	1.073%
60	15.315	2244	2249	2252	rBV	937929	1144526	21.69%	2.419%
61	15.339	2252	2253	2256	rVB	108773	75378	1.43%	0.159%
62	15.780	2324	2328	2334	rBV3	95056	148673	2.82%	0.314%
63	16.680	2476	2481	2492	rVB2	186586	387667	7.35%	0.819%
64	17.098	2546	2552	2562	rVB	136158	292401	5.54%	0.618%

Sum of corrected areas: 47307181

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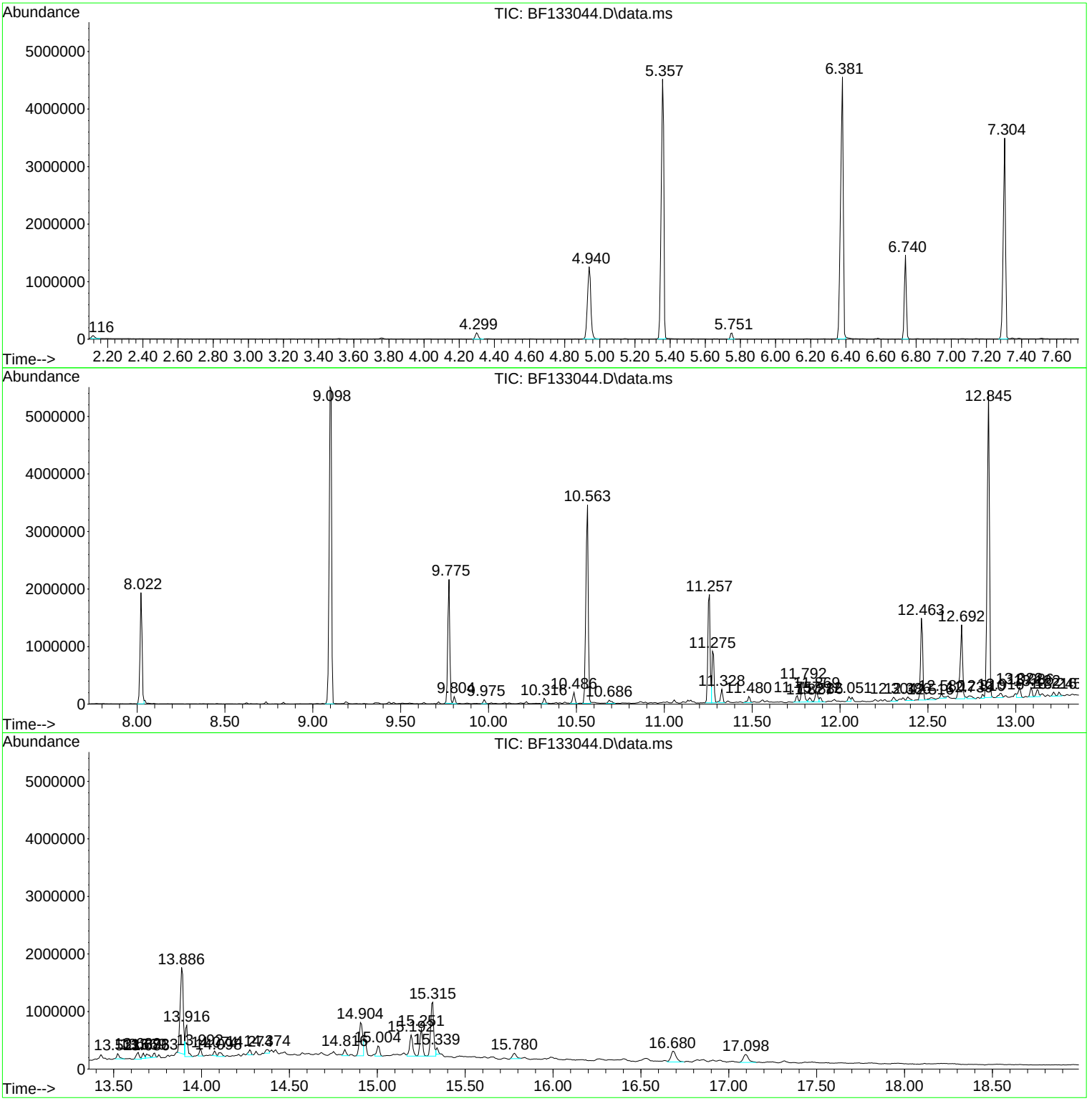
ClientSampleId :
SB-19-0-2-20230411

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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\BF042523\
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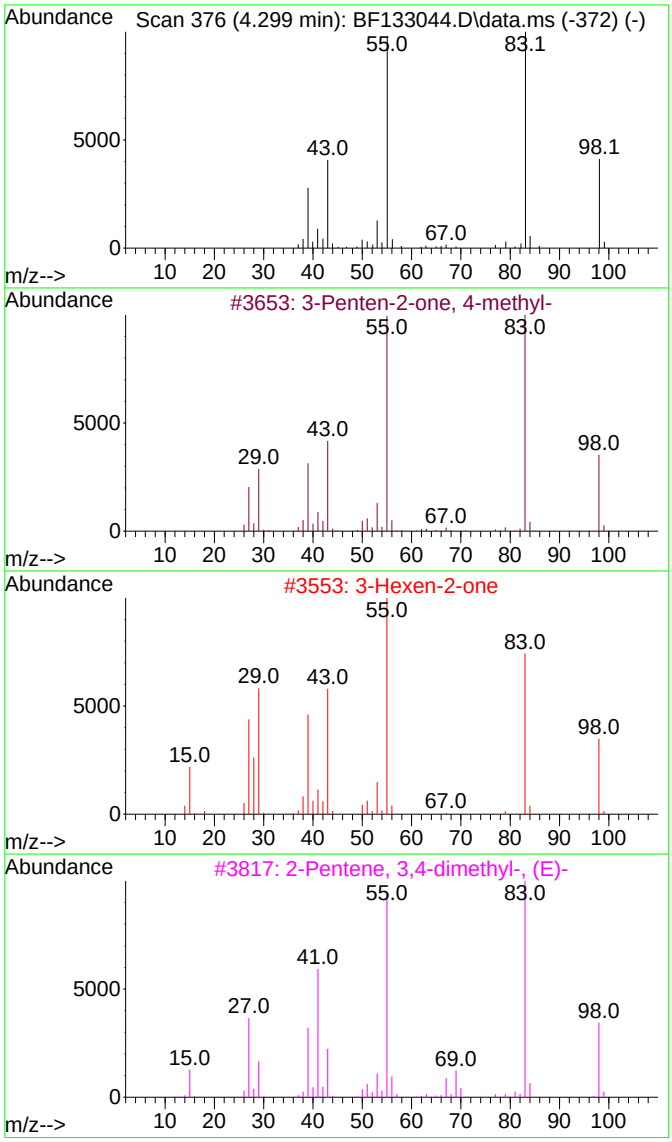
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

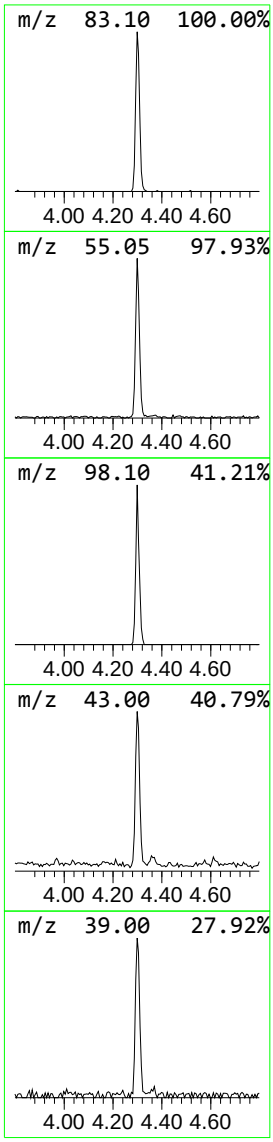
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.299	2.18 ng	124493	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	94
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	Cyclohexane, methyl-	98	C7H14	000108-87-2	80





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Instrument :
BNA_F
ClientSampleId :
SB-19-0-2-20230411

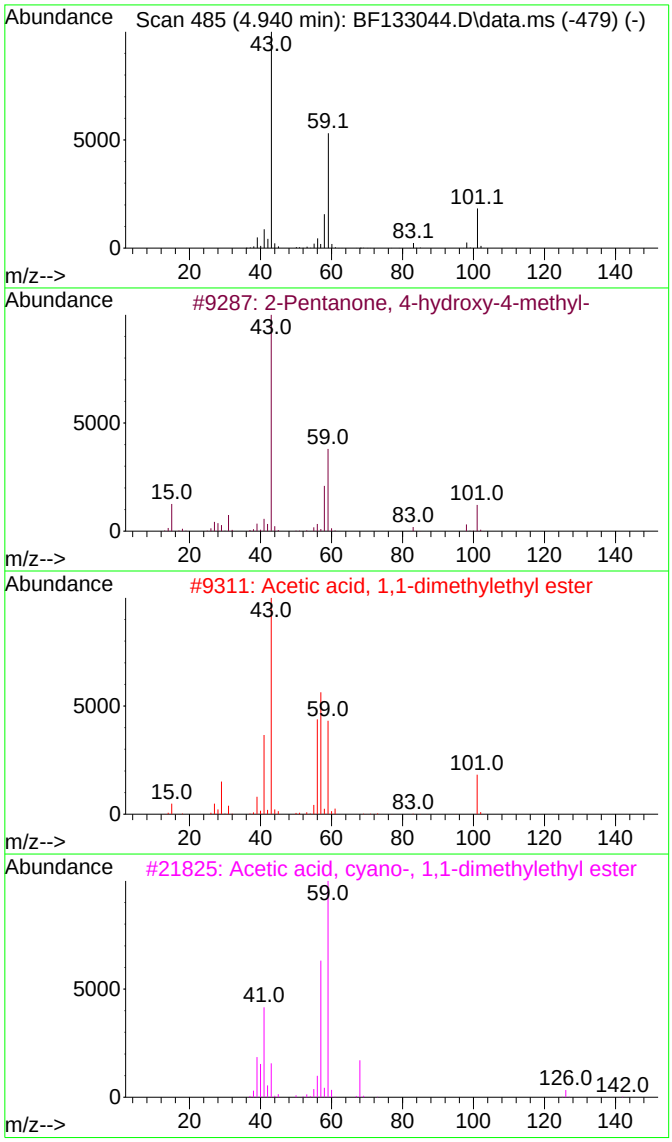
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

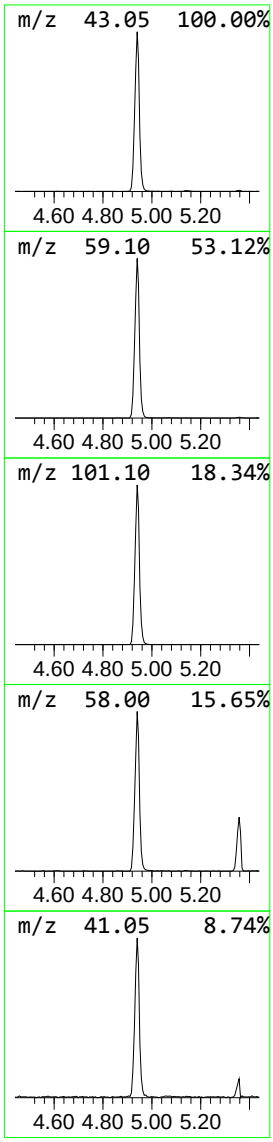
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.940	28.92 ng	1653500	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	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

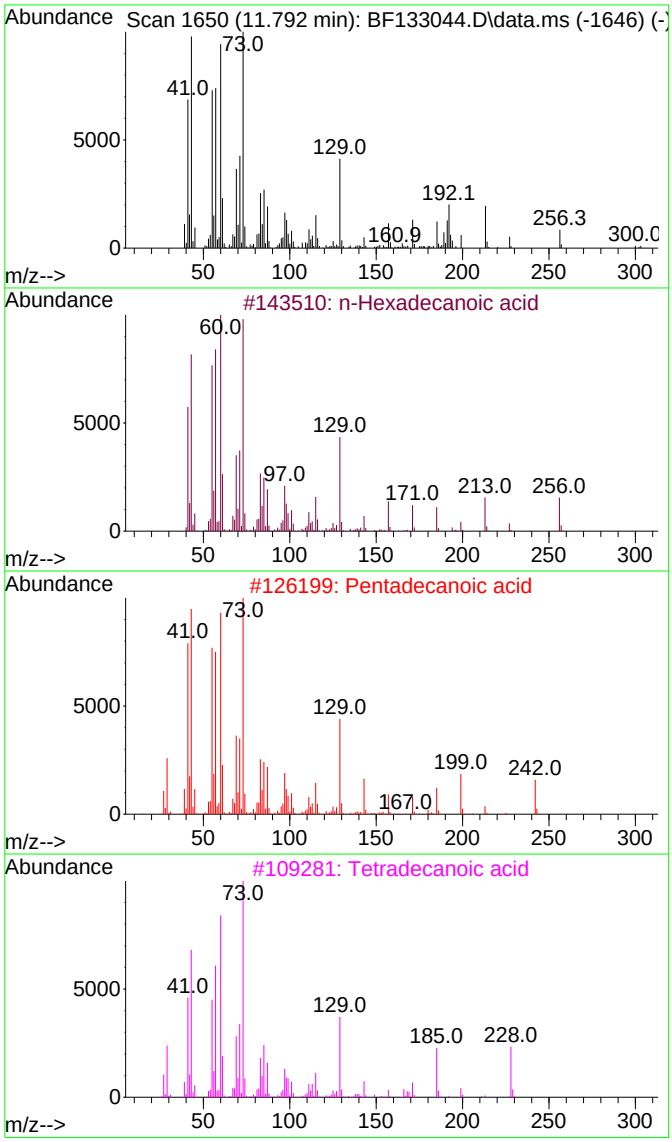
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

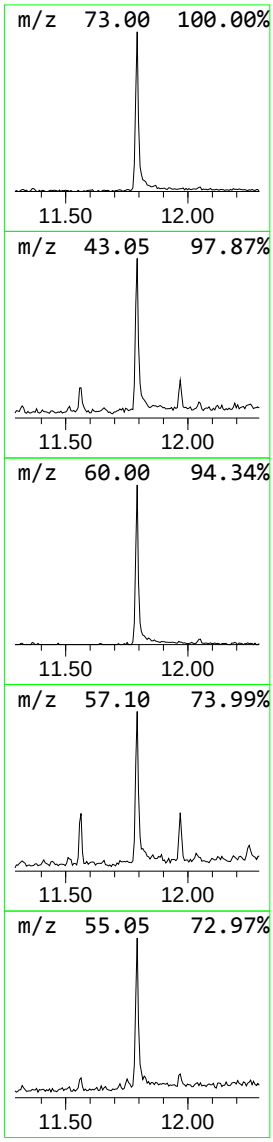
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.792	4.74 ng	415599	Phenanthrene-d10	11.257

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tridecanoic acid	214	C13H26O2	000638-53-9	70





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ClientSampleId :
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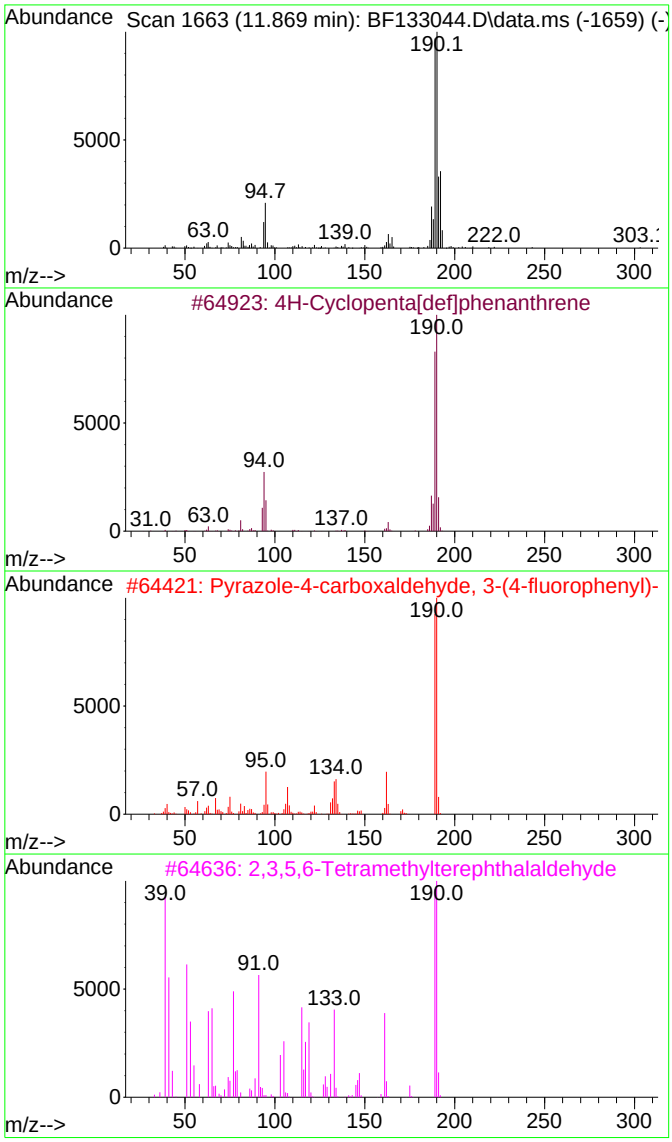
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

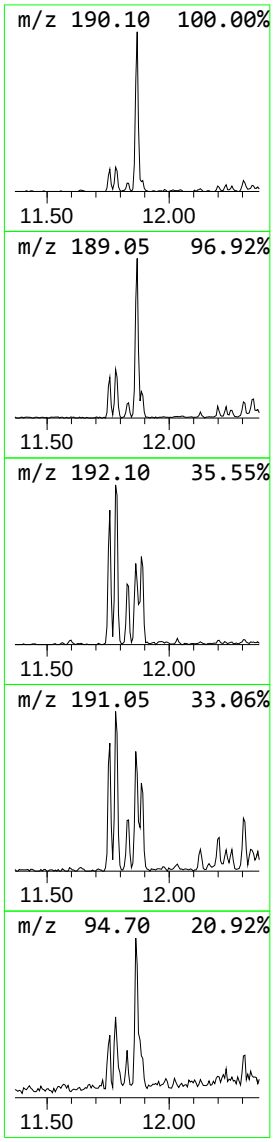
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.869	2.28 ng	200288	Phenanthrene-d10	11.257

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	91
2	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	52
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	47
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	35





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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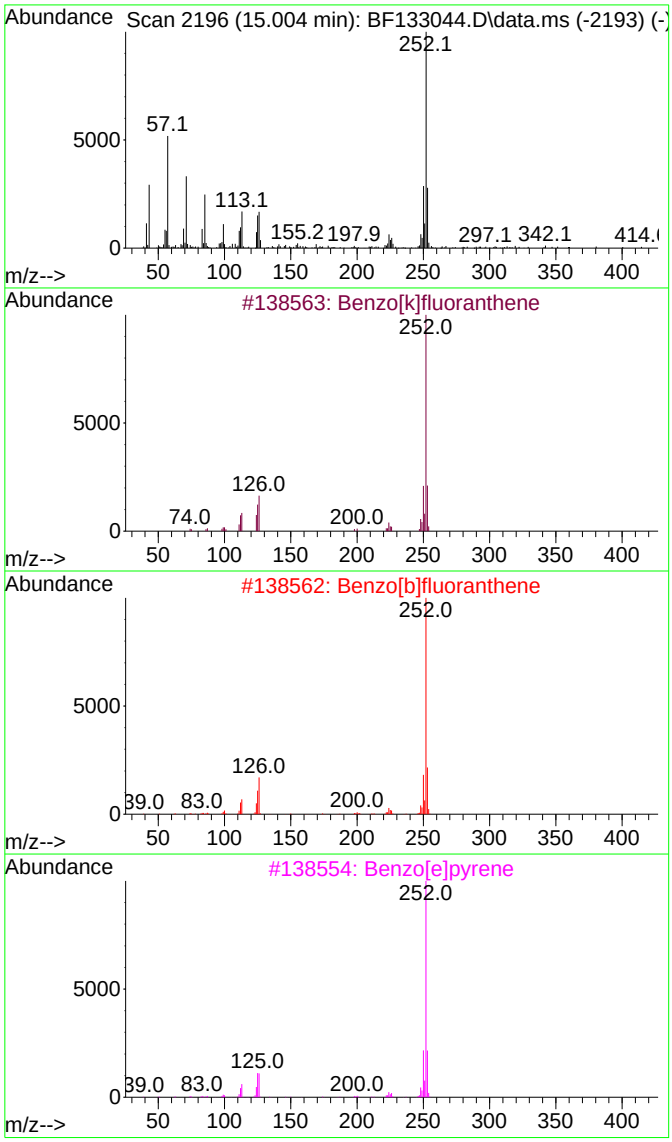
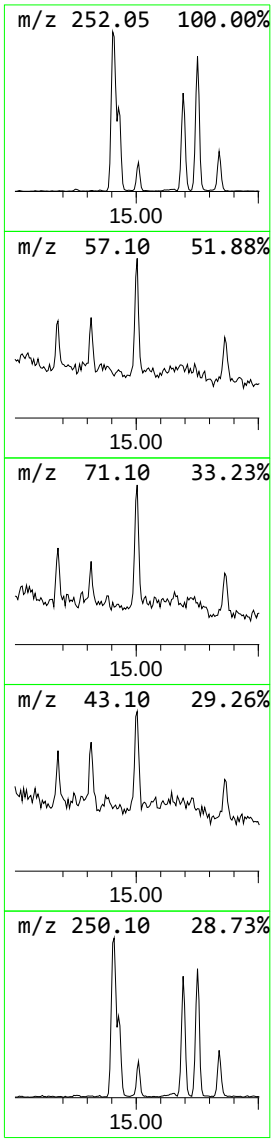
Peak Number 5 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.004	3.50 ng	200309	Perylene-d12	15.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
3	Benzo[e]pyrene	252	C20H12	000192-97-2	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	86





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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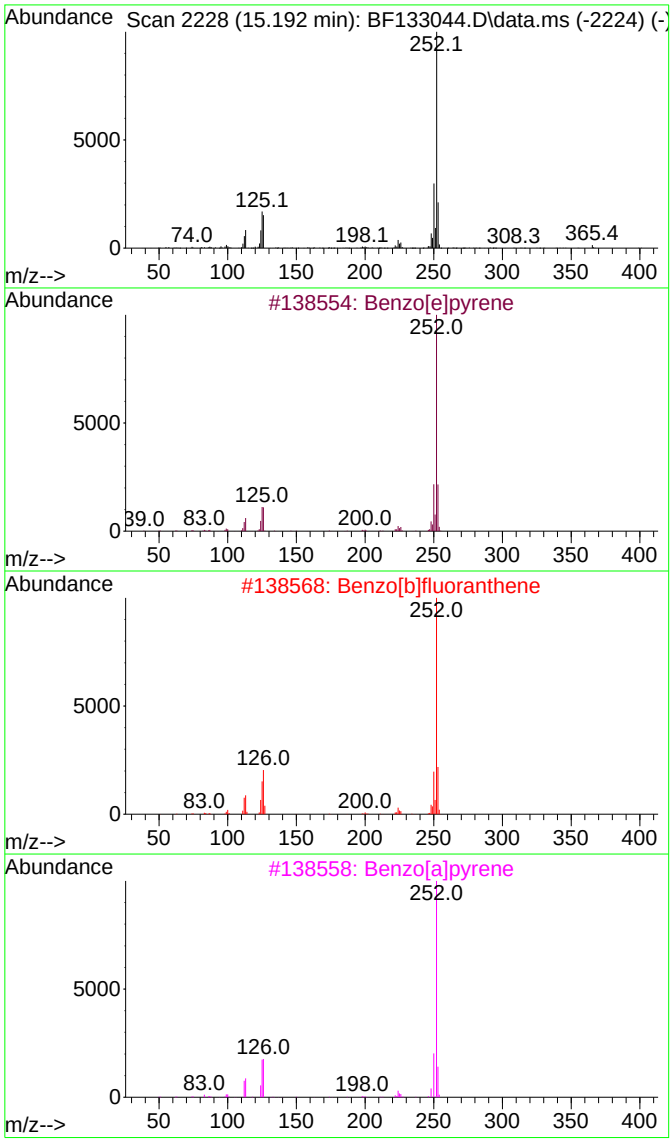
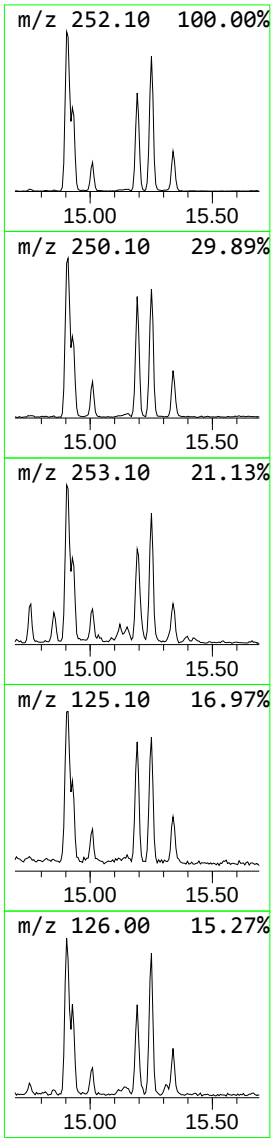
Peak Number 6 Benzo[j]fluoranthene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.192	7.85 ng	449236	Perylene-d12	15.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
3	Benzo[a]pyrene	252	C20H12	000050-32-8	93
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90





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Data File : BF133044.D
Acq On : 26 Apr 2023 00:02
Operator : CG\JU
Sample : 02270-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-19-0-2-20230411

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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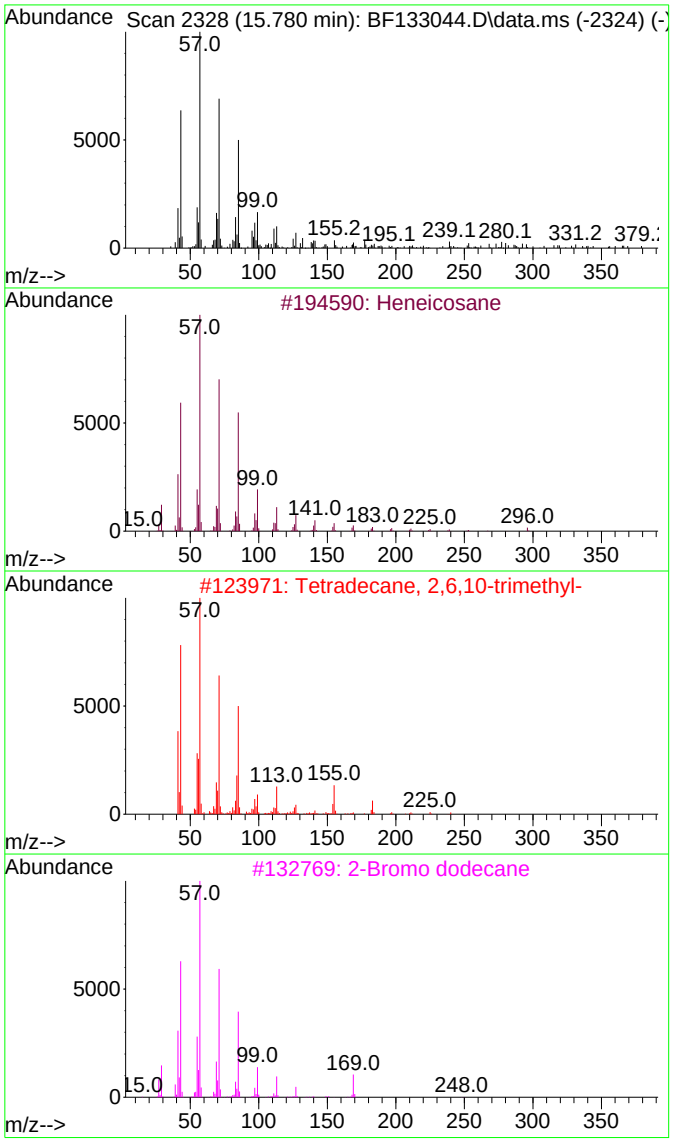
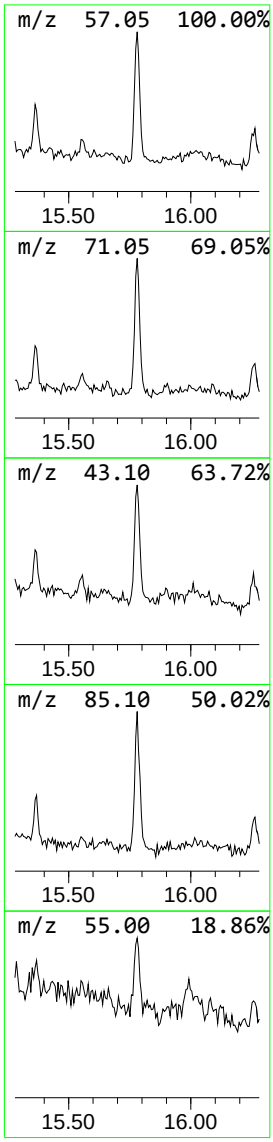
Peak Number 7 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.780	2.60 ng	148673	Perylene-d12	15.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	93
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
4	Nonadecane	268	C19H40	000629-92-5	91
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133044.D
Acq On : 26 Apr 2023 00:02
Operator : CG\JU
Sample : 02270-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-19-0-2-20230411

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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,...	4.299	2.2	ng	124493	1	6.740	1143350	20.0
2-Pentanone, 4-...	4.940	28.9	ng	1653500	1	6.740	1143350	20.0
n-Hexadecanoic ...	11.792	4.7	ng	415599	4	11.257	1753080	20.0
4H-Cyclopenta[d...	11.869	2.3	ng	200288	4	11.257	1753080	20.0
Benzo[e]pyrene	15.004	3.5	ng	200309	6	15.316	1144530	20.0
Benzo[j]fluoran...	15.192	7.8	ng	449236	6	15.316	1144530	20.0
Heneicosane	15.780	2.6	ng	148673	6	15.316	1144530	20.0