LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
Data File : BF122441.D
Acq On : 22 Nov 2020 2:09
Operator : JU/CG
Sample : L4845-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PH-TP

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-BF110920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122441.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	5	10	18	rVB	382457	491284	9.28%	1.011%
2	2.252	25	28	43	rVB3	48808	93042	1.76%	0.191%
3	5.075	502	508	519	rVB	706932	862052	16.28%	1.774%
4	5.487	573	578	581	rBV	4049892	3794887	71.67%	7.810%
5	5.875	641	644	651	rVB	97530	82274	1.55%	0.169%
6	6.493	744	749	762	rBV	3678343	4131564	78.03%	8.503%
7	6.863	808	812	815	rBV	1479699	1173385	22.16%	2.415%
8	7.422	902	907	910	rBV	2512461	2544815	48.06%	5.238%
9	8.151	1026	1031	1034	rBV	1551167	1520345	28.71%	3.129%
10	9.228	1209	1214	1217	rBV	5288854	4569890	86.31%	9.405%
11	9.345	1230	1234	1244	rVB	268250	264314	4.99%	0.544%
12	9.622	1277	1281	1289	rVB	225427	229671	4.34%	0.473%
13	9.904	1325	1329	1333	rBV	1999566	1822622	34.42%	3.751%
14	9.939	1333	1335	1339	rVB	85361	71480	1.35%	0.147%
15	10.451	1419	1422	1426	rBV	83764	77521	1.46%	0.160%
16	10.692	1459	1463	1479	rBV	3095969	3268333	61.73%	6.727%
17	11.257	1552	1559	1562	rBV4	60068	80021	1.51%	0.165%
18	11.392	1578	1582	1584	rBV	2109051	1931841	36.49%	3.976%
19	11.416	1584	1586	1590	rVV	1217427	1004657	18.97%	2.068%
20	11.469	1590	1595	1599	rVB	230005	237271	4.48%	0.488%
21	11.622	1616	1621	1630	rBV2	160937	207224	3.91%	0.426%
22	11.898	1664	1668	1670	rBV	102257	100633	1.90%	0.207%
23	11.922	1670	1672	1677	rVB	278719	241737	4.57%	0.498%
24	12.010	1683	1687	1689	rBV	204761	208254	3.93%	0.429%
25	12.027	1689	1690	1695	rVB	77349	70511	1.33%	0.145%
26	12.192	1713	1718	1720	rBV	80121	72417	1.37%	0.149%
27	12.445	1758	1761	1764	rBV	54506	57009	1.08%	0.117%
28	12.486	1764	1768	1773	rVB4	58271	80095	1.51%	0.165%
29	12.610	1785	1789	1792	rBV	1767996	1499481	28.32%	3.086%
30	12.839	1821	1828	1830	rBV	1305669	1388420	26.22%	2.858%
31	12.886	1834	1836	1841	rVB2	78200	71819	1.36%	0.148%
32	12.957	1845	1848	1849	rBV	87855	75319	1.42%	0.155%
33	12.986	1849	1853	1856	rVV	5687690	5294811	100.00%	10.897%
34	13.057	1860	1865	1868	rBV2	78974	128294	2.42%	0.264%
35	13.169	1873	1884	1887	rBV	306305	426543	8.06%	0.878%
36	13.233	1891	1895	1898	rBV	262901	227900	4.30%	0.469%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
Data File : BF122441.D
Acq On : 22 Nov 2020 2:09
Operator : JU/CG
Sample : L4845-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PH-TP

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-BF110920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.269	1898	1901	1904	rBV	120855	115885	2.19%	0.239%
38	13.363	1914	1917	1920	rVB	69532	62969	1.19%	0.130%
39	13.392	1920	1922	1926	rBV2	86641	91721	1.73%	0.189%
40	13.563	1946	1951	1954	rBV3	93360	143495	2.71%	0.295%
41	13.674	1968	1970	1975	rVB2	62517	81991	1.55%	0.169%
42	13.786	1985	1989	1992	rBV2	114352	138863	2.62%	0.286%
43	13.816	1992	1994	1996	rVV	98408	74351	1.40%	0.153%
44	13.886	2003	2006	2013	rVB2	329941	442192	8.35%	0.910%
45	14.039	2024	2032	2035	rBV2	2405513	2923517	55.21%	6.017%
46	14.063	2035	2036	2042	rVB	790541	542859	10.25%	1.117%
47	14.145	2047	2050	2052	rVB	91139	74687	1.41%	0.154%
48	14.210	2058	2061	2063	rBV2	75243	80415	1.52%	0.166%
49	14.263	2066	2070	2073	rVB2	65272	91485	1.73%	0.188%
50	14.427	2093	2098	2101	rBV	124907	134342	2.54%	0.276%
51	14.457	2101	2103	2107	rVB2	73727	69731	1.32%	0.144%
52	14.516	2108	2113	2117	rBV3	142590	209472	3.96%	0.431%
53	14.569	2120	2122	2126	rVB2	99873	109025	2.06%	0.224%
54	14.827	2163	2166	2169	rVB2	52192	55487	1.05%	0.114%
55	14.904	2176	2179	2186	rBV2	104133	160911	3.04%	0.331%
56	15.086	2205	2210	2213	rBV	528110	849534	16.04%	1.748%
57	15.168	2221	2224	2226	rBV3	64817	77967	1.47%	0.160%
58	15.192	2226	2228	2233	rVB	94366	95986	1.81%	0.198%
59	15.392	2258	2262	2268	rVB	286468	377765	7.13%	0.777%
60	15.451	2268	2272	2278	rVB	435807	510281	9.64%	1.050%
61	15.516	2278	2283	2287	rBV	1263397	1606833	30.35%	3.307%
62	16.004	2362	2366	2370	rBV2	53130	81387	1.54%	0.168%
63	16.074	2372	2378	2383	rVB6	43723	114917	2.17%	0.237%
64	16.804	2498	2502	2514	rVB3	36517	92210	1.74%	0.190%
65	16.986	2527	2533	2543	rVB2	174865	366629	6.92%	0.755%
66	17.168	2559	2564	2568	rBV	29884	62724	1.18%	0.129%
67	17.427	2602	2608	2619	rVB	125997	279326	5.28%	0.575%
68	17.662	2644	2648	2654	rVB	38042	66811	1.26%	0.138%

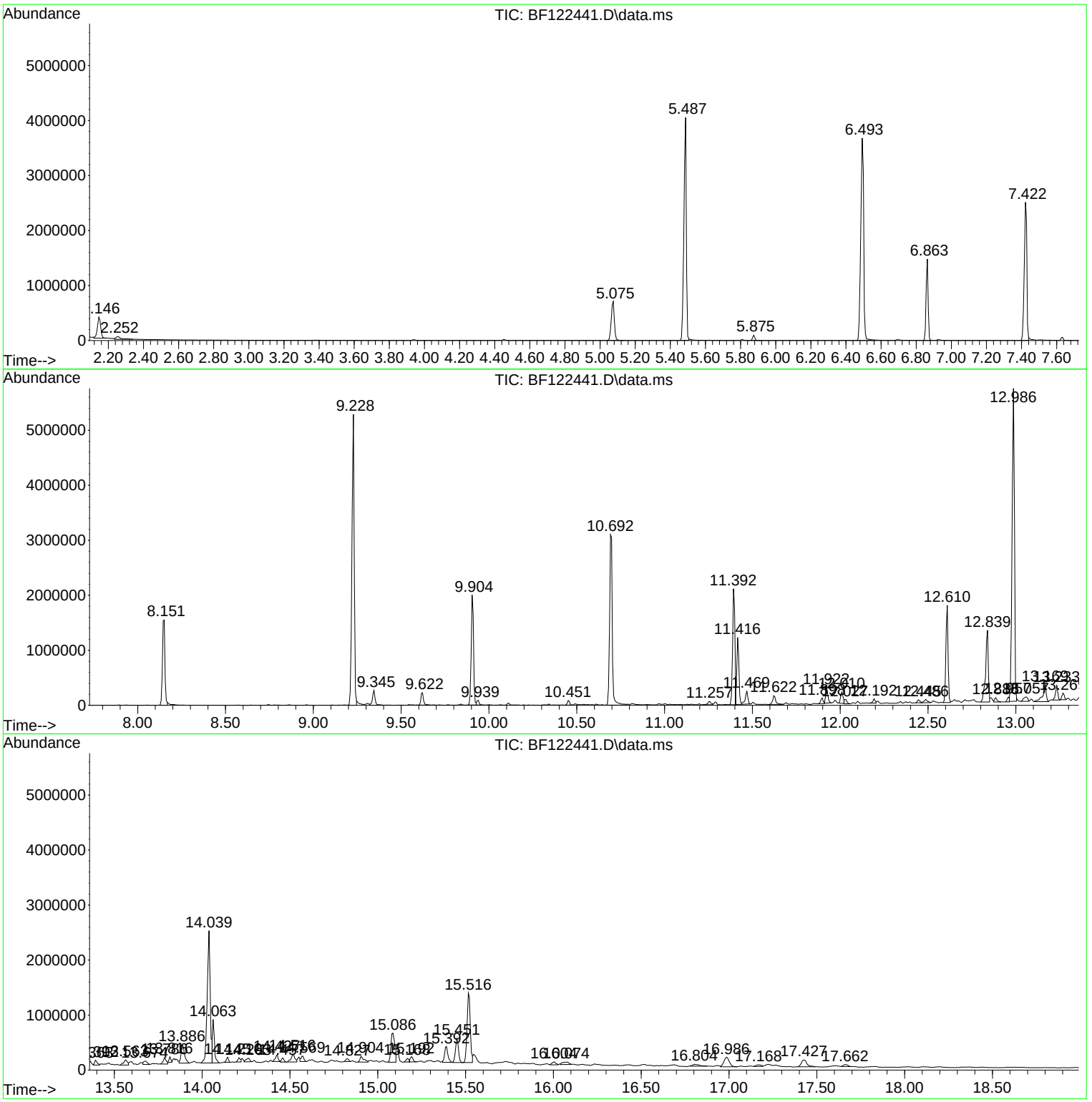
Sum of corrected areas: 48587504

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
Data File : BF122441.D
Acq On : 22 Nov 2020 2:09
Operator : JU/CG
Sample : L4845-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PH-TP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
Data File : BF122441.D
Acq On : 22 Nov 2020 2:09
Operator : JU/CG
Sample : L4845-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PH-TP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

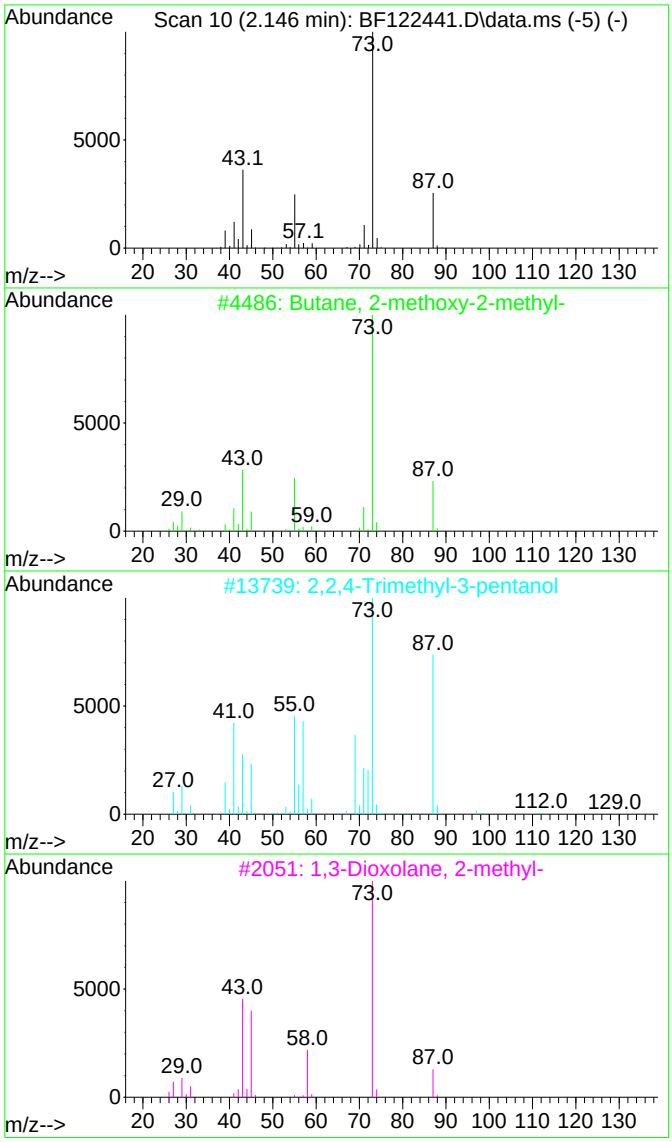
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

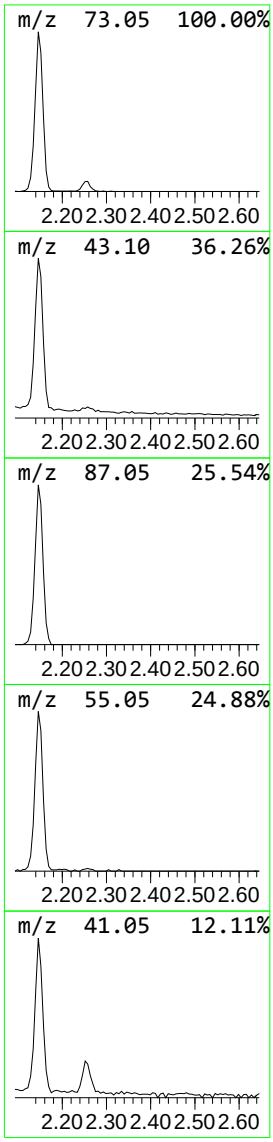
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	8.37 ng	491284	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
Data File : BF122441.D
Acq On : 22 Nov 2020 2:09
Operator : JU/CG
Sample : L4845-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PH-TP

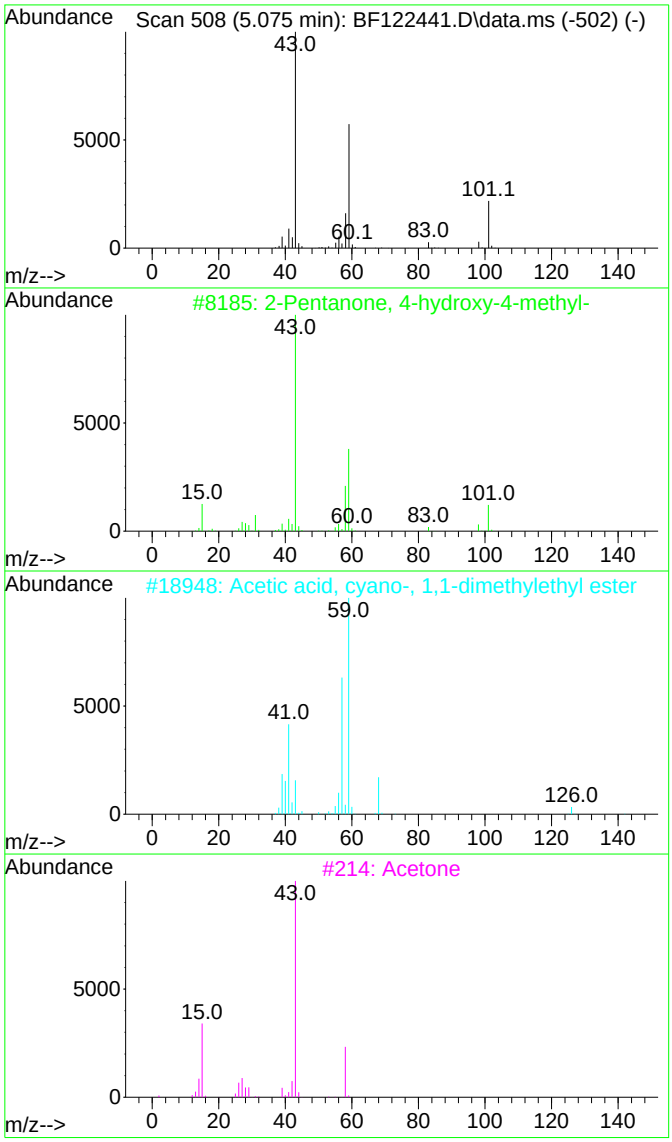
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

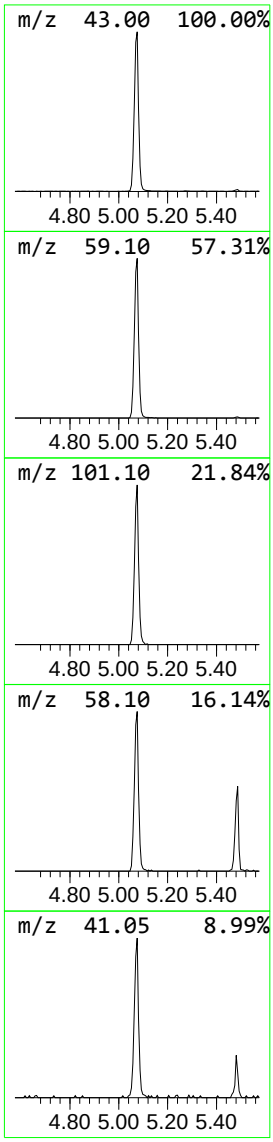
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	14.69 ng	862052	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	Acetone	58	C3H6O	000067-64-1	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
Data File : BF122441.D
Acq On : 22 Nov 2020 2:09
Operator : JU/CG
Sample : L4845-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PH-TP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

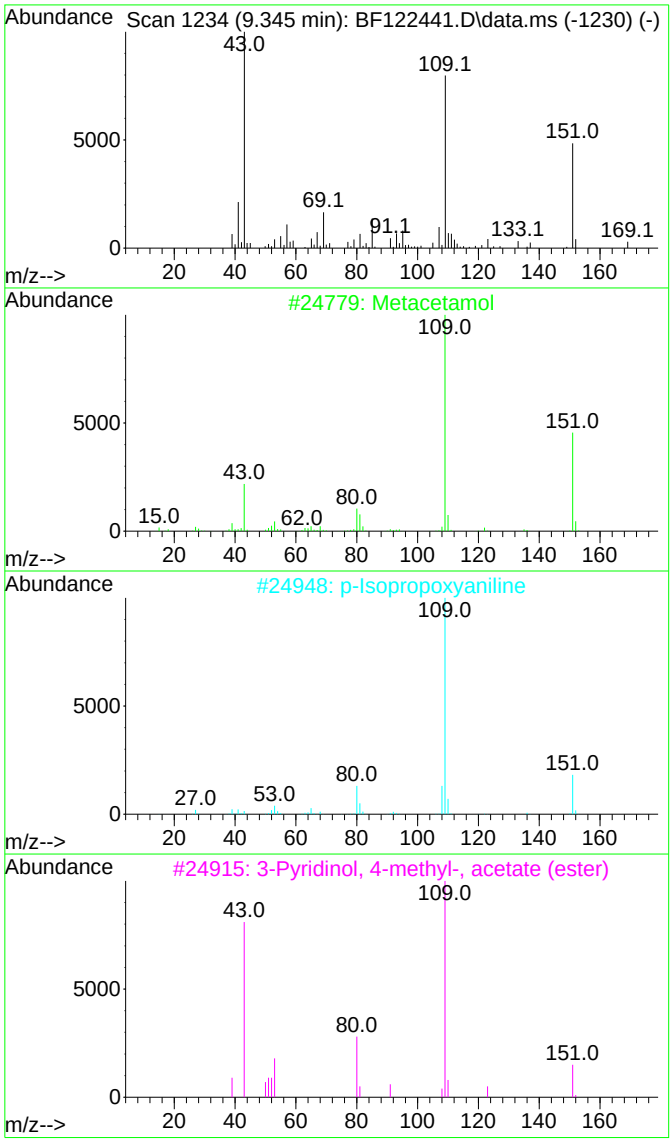
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

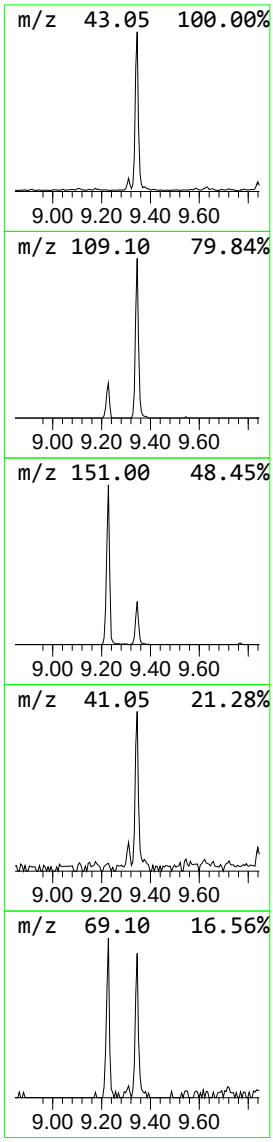
****

Peak Number 3 Metacetamol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.345	2.90 ng	264314	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Metacetamol	151	C8H9NO2	000621-42-1	59
2	p-Isopropoxyaniline	151	C9H13NO	007664-66-6	59
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	59
5	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
Data File : BF122441.D
Acq On : 22 Nov 2020 2:09
Operator : JU/CG
Sample : L4845-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PH-TP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

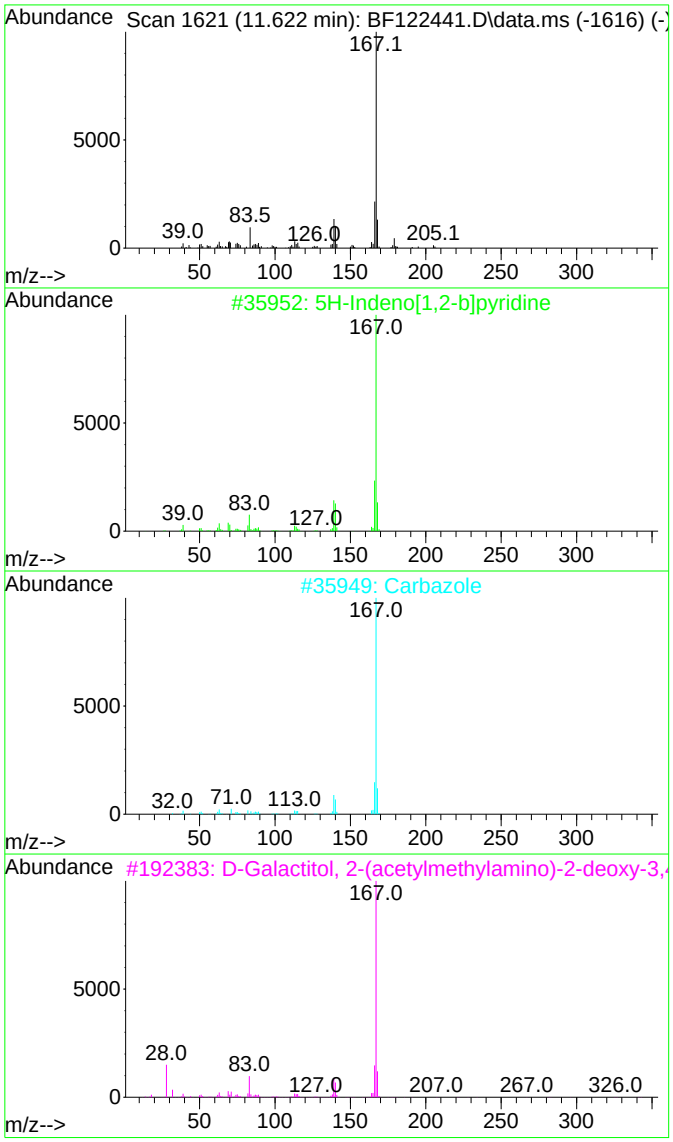
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

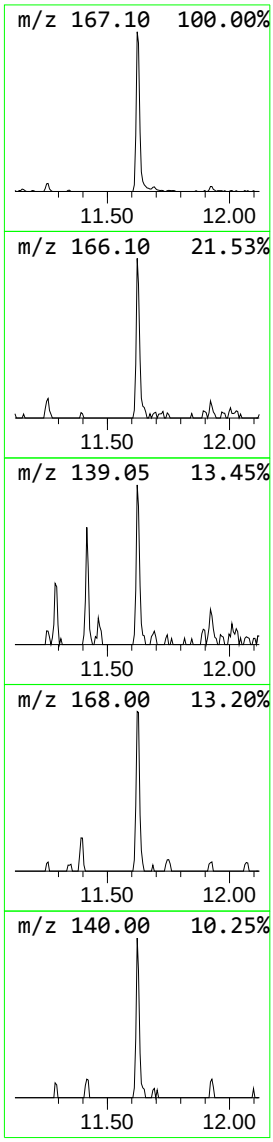
****

Peak Number 5 5H-Indeno[1,2-b]pyridine Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.622	2.15 ng	207224	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	95
2	Carbazole	167	C12H9N	000086-74-8	93
3	D-Galactitol, 2-(acetylmethylami...	363	C16H29NO8	074410-42-7	87
4	9H-Carbazole, 9-nitroso-	196	C12H8N2O	002788-23-0	83
5	1,1'-Biphenyl, 2-azido-	195	C12H9N3	007599-23-7	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
Data File : BF122441.D
Acq On : 22 Nov 2020 2:09
Operator : JU/CG
Sample : L4845-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PH-TP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

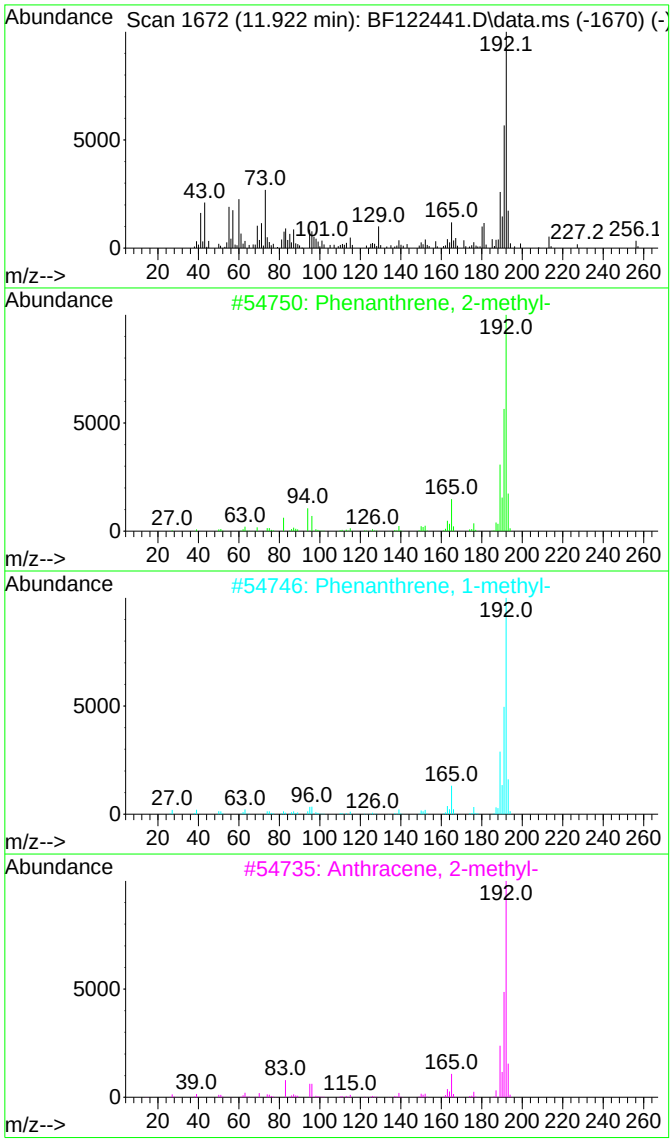
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

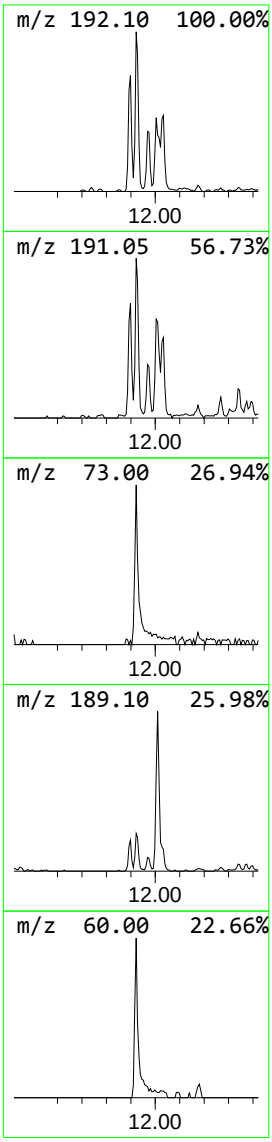
****

Peak Number 6 Phenanthrene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	2.50 ng	241737	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
Data File : BF122441.D
Acq On : 22 Nov 2020 2:09
Operator : JU/CG
Sample : L4845-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PH-TP

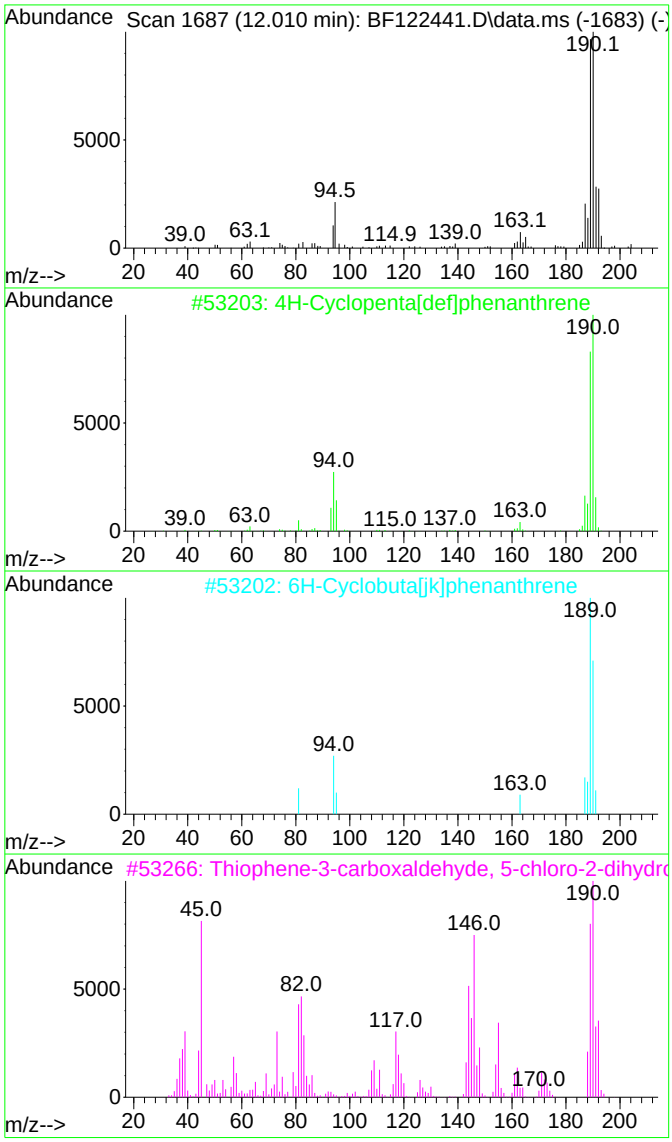
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

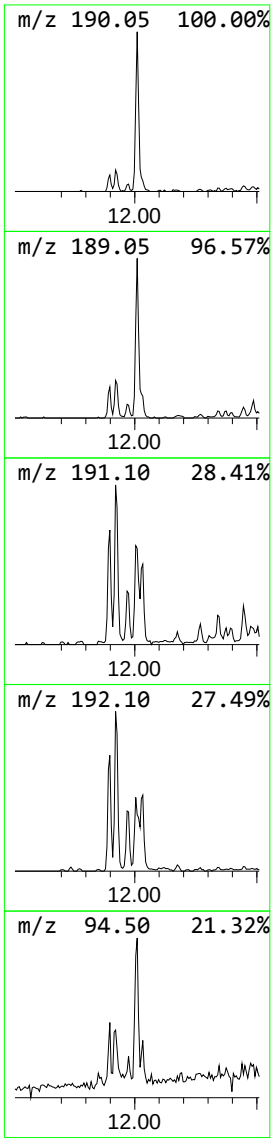
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	2.16 ng	208254	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	56
3	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	52
4	Methyl diselenide	190	C2H6Se2	007101-31-7	49
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
Data File : BF122441.D
Acq On : 22 Nov 2020 2:09
Operator : JU/CG
Sample : L4845-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PH-TP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

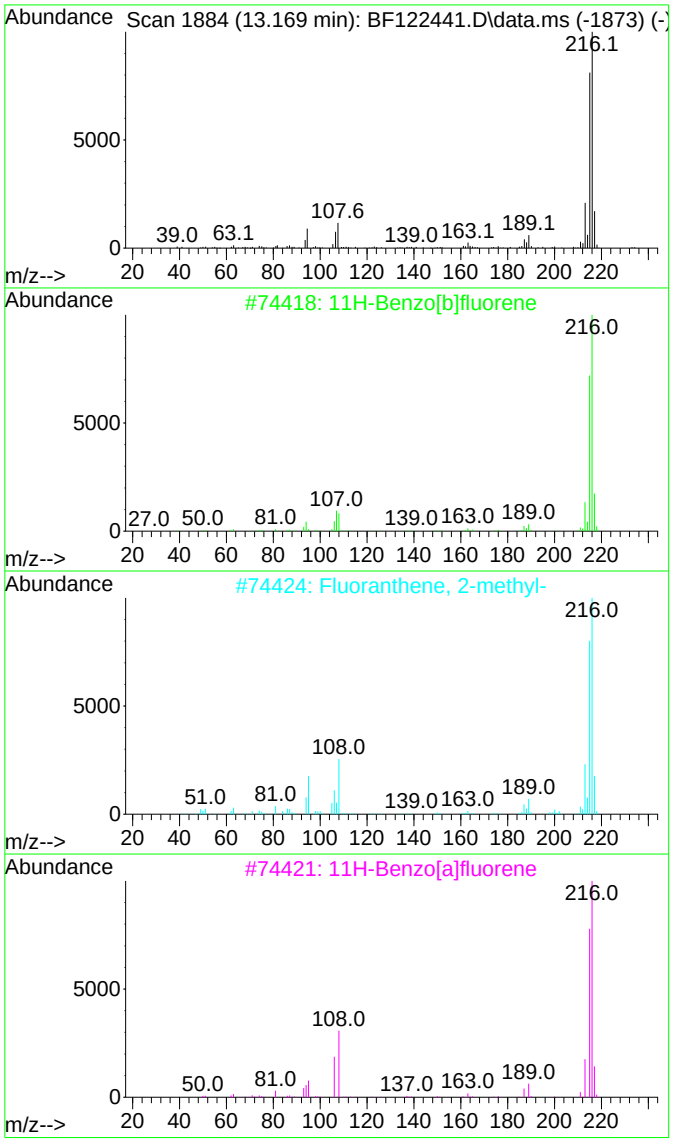
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

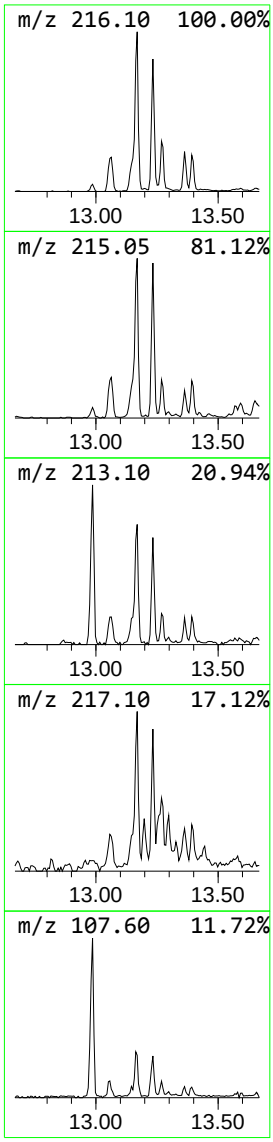
****

Peak Number 8 11H-Benzo[b]fluorene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.169	2.92 ng	426543	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	96
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	94
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
Data File : BF122441.D
Acq On : 22 Nov 2020 2:09
Operator : JU/CG
Sample : L4845-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PH-TP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

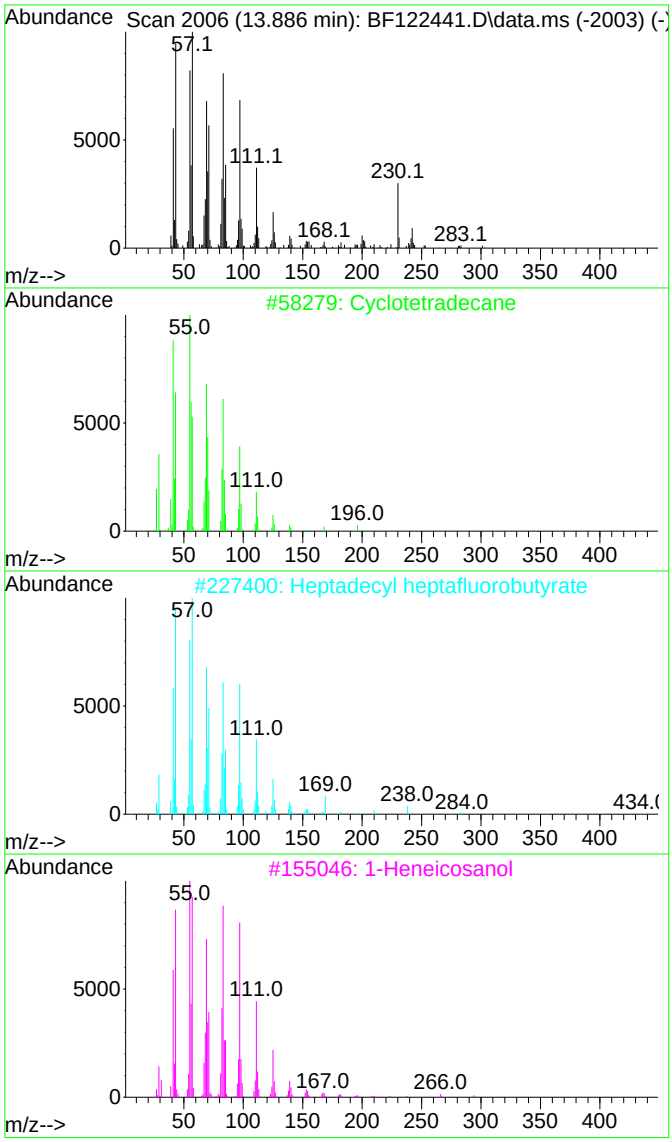
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

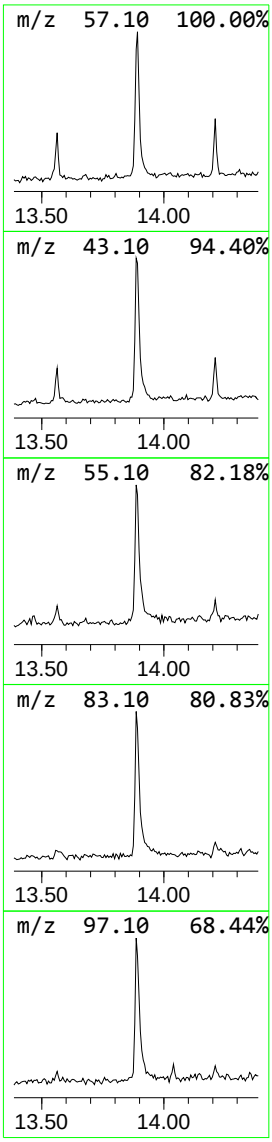
****

Peak Number 9 Cyclotetradecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	3.03 ng	442192	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	96
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
Data File : BF122441.D
Acq On : 22 Nov 2020 2:09
Operator : JU/CG
Sample : L4845-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PH-TP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

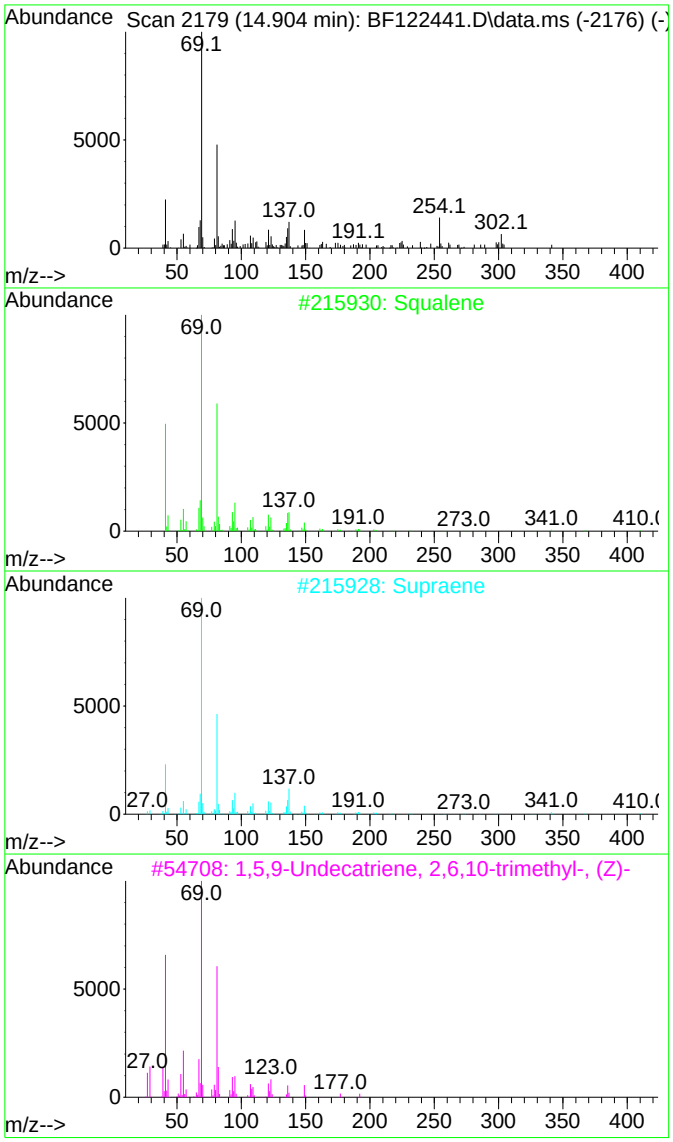
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

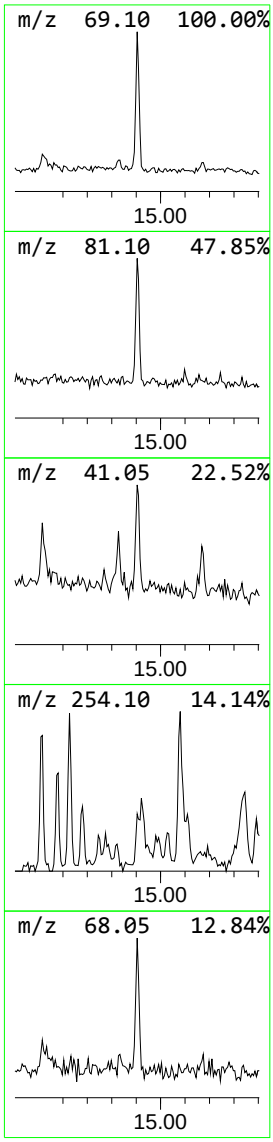
****

Peak Number 10 Squalene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	2.00 ng	160911	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	81
2	Supraene	410	C30H50	007683-64-9	81
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	59
5	1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
Data File : BF122441.D
Acq On : 22 Nov 2020 2:09
Operator : JU/CG
Sample : L4845-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PH-TP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

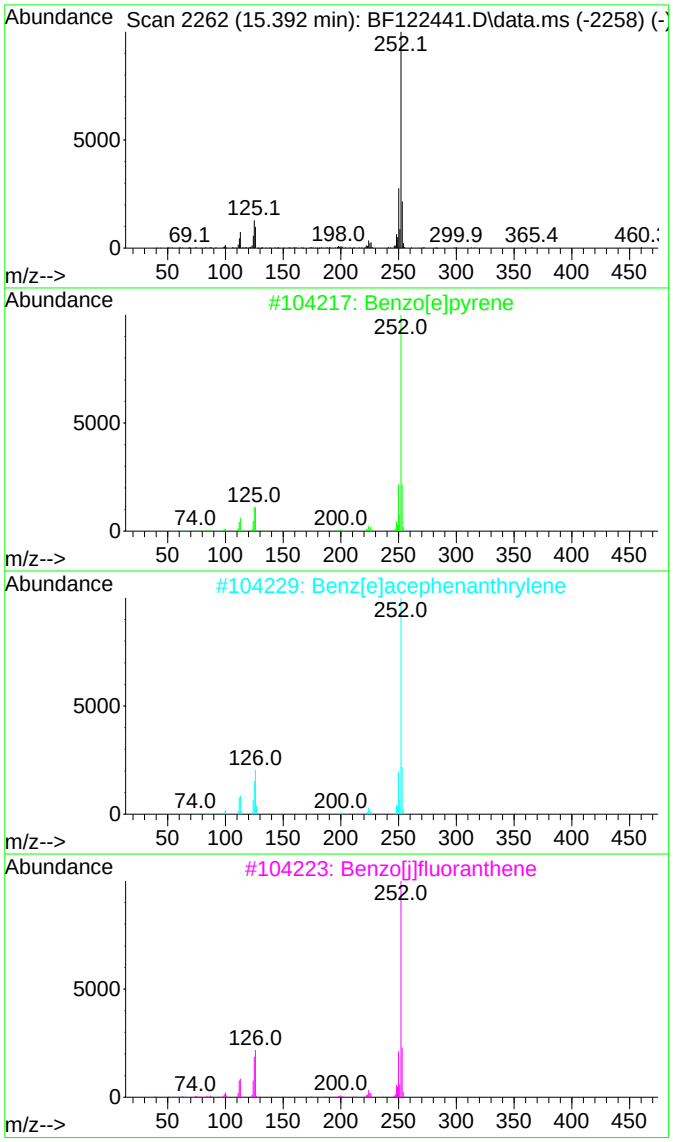
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

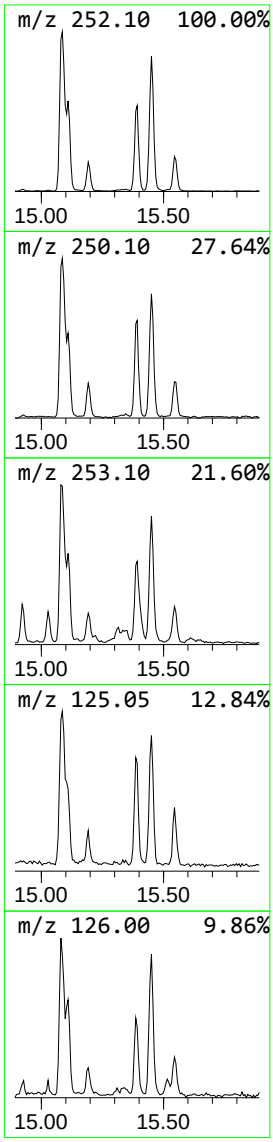
****

Peak Number 11 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.392	4.70 ng	377765	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Perylene	252	C20H12	000198-55-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
Data File : BF122441.D
Acq On : 22 Nov 2020 2:09
Operator : JU/CG
Sample : L4845-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PH-TP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.146	8.4	ng	491284	1	6.863	1173390	20.0
2-Pentanone, 4-...	5.075	14.7	ng	862052	1	6.863	1173390	20.0
Metacetamol	9.345	2.9	ng	264314	3	9.904	1822620	20.0
5H-Indeno[1,2-b...	11.622	2.1	ng	207224	4	11.392	1931840	20.0
Phenanthrene, 2...	11.922	2.5	ng	241737	4	11.392	1931840	20.0
4H-Cyclopenta[d...	12.010	2.2	ng	208254	4	11.392	1931840	20.0
11H-Benzo[b]flu...	13.169	2.9	ng	426543	5	14.039	2923520	20.0
Cyclotetradecane	13.886	3.0	ng	442192	5	14.039	2923520	20.0
Squalene	14.904	2.0	ng	160911	6	15.515	1606830	20.0
Benzo[e]pyrene	15.392	4.7	ng	377765	6	15.515	1606830	20.0