LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092521\
Data File : BF125664.D
Acq On : 25 Sep 2021 19:08
Operator : JU/CG
Sample : M3943-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-DB-1

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-BF092421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125664.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	9	15	21	rVB	1088109	1371220	36.95%	3.713%
2	5.104	505	513	520	rBV	53283	71141	1.92%	0.193%
3	5.504	576	581	584	rBV	3151617	2844825	76.66%	7.704%
4	6.504	746	751	754	rBV	2940921	2845970	76.70%	7.707%
5	6.886	812	816	819	rBV	1931687	1465958	39.51%	3.970%
6	7.445	906	911	914	rBV	2072066	1837472	49.52%	4.976%
7	8.069	1013	1017	1020	rBV	1489096	1160656	31.28%	3.143%
8	8.169	1030	1034	1037	rBV	2526074	1991862	53.68%	5.394%
9	9.245	1212	1217	1220	rBV	4012576	3710735	100.00%	10.049%
10	9.357	1233	1236	1244	rVB	402214	348276	9.39%	0.943%
11	9.921	1328	1332	1335	rBV	2820229	2233710	60.20%	6.049%
12	10.104	1360	1363	1371	rVB2	90500	95956	2.59%	0.260%
13	10.410	1412	1415	1422	rVB	223976	193462	5.21%	0.524%
14	10.668	1455	1459	1462	rBV2	129948	132767	3.58%	0.360%
15	10.704	1462	1465	1469	rVB	2223476	1971514	53.13%	5.339%
16	11.404	1580	1584	1587	rBV	2266733	2001762	53.95%	5.421%
17	11.427	1587	1588	1591	rVV	363441	201999	5.44%	0.547%
18	11.480	1594	1597	1599	rVB	69074	63802	1.72%	0.173%
19	11.798	1648	1651	1659	rBV	108188	92895	2.50%	0.252%
20	11.904	1666	1669	1671	rBV	60316	59185	1.59%	0.160%
21	11.927	1671	1673	1680	rVB2	466329	426342	11.49%	1.155%
22	12.015	1685	1688	1691	rBV2	84263	91674	2.47%	0.248%
23	12.198	1714	1719	1721	rBV	46782	47712	1.29%	0.129%
24	12.457	1759	1763	1765	rBV	50293	53906	1.45%	0.146%
25	12.504	1768	1771	1774	rVV	332153	272261	7.34%	0.737%
26	12.533	1774	1776	1783	rVB3	37757	46408	1.25%	0.126%
27	12.592	1783	1786	1787	rBV	100001	79035	2.13%	0.214%
28	12.615	1787	1790	1794	rVB	554448	452901	12.21%	1.226%
29	12.715	1804	1807	1814	rBV2	106964	141246	3.81%	0.382%
30	12.845	1823	1829	1832	rBV	557623	513866	13.85%	1.392%
31	12.986	1849	1853	1857	rVB	2945752	2671529	71.99%	7.235%
32	13.062	1861	1866	1870	rVB4	30307	46445	1.25%	0.126%
33	13.168	1882	1884	1887	rVB3	52821	52943	1.43%	0.143%
34	13.221	1888	1893	1894	rBV5	36299	48985	1.32%	0.133%
35	13.274	1900	1902	1905	rVB2	49652	39745	1.07%	0.108%
36	13.398	1921	1923	1927	rBV2	40902	49775	1.34%	0.135%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092521\
Data File : BF125664.D
Acq On : 25 Sep 2021 19:08
Operator : JU/CG
Sample : M3943-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-DB-1

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-BF092421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.439	1927	1930	1932	rVV	123099	98814	2.66%	0.268%
38	13.462	1932	1934	1940	rVV4	26419	46569	1.25%	0.126%
39	13.533	1940	1946	1947	rVV2	111280	166348	4.48%	0.450%
40	13.574	1948	1953	1968	rVV2	223857	1146057	30.88%	3.104%
41	13.674	1968	1970	1979	rVB	88909	112369	3.03%	0.304%
42	13.792	1985	1990	1992	rBV2	36655	56699	1.53%	0.154%
43	13.880	2002	2005	2007	rBV2	44164	51361	1.38%	0.139%
44	14.039	2024	2032	2035	rBV2	1811684	1896253	51.10%	5.135%
45	14.062	2035	2036	2042	rVB	238975	207514	5.59%	0.562%
46	14.127	2044	2047	2049	rBV2	65631	55635	1.50%	0.151%
47	14.427	2095	2098	2101	rVB	53810	54546	1.47%	0.148%
48	14.803	2158	2162	2164	rBV	80176	95544	2.57%	0.259%
49	14.903	2176	2179	2186	rVB5	36317	57342	1.55%	0.155%
50	15.080	2205	2209	2213	rBV	215084	362856	9.78%	0.983%
51	15.168	2220	2224	2226	rBV2	54041	69026	1.86%	0.187%
52	15.386	2257	2261	2267	rVB	147472	177226	4.78%	0.480%
53	15.450	2267	2272	2276	rVV	203763	254265	6.85%	0.689%
54	15.515	2278	2283	2287	rVV2	1325543	1718693	46.32%	4.654%
55	15.550	2287	2289	2297	rVB3	117006	149016	4.02%	0.404%
56	15.998	2361	2365	2370	rBV3	64995	85408	2.30%	0.231%
57	16.515	2449	2453	2458	rBV2	42826	68345	1.84%	0.185%
58	16.986	2528	2533	2542	rVB2	74309	154619	4.17%	0.419%
59	17.433	2604	2609	2617	rVB2	56649	112697	3.04%	0.305%

Sum of corrected areas: 36927142

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Operator : JU/CG
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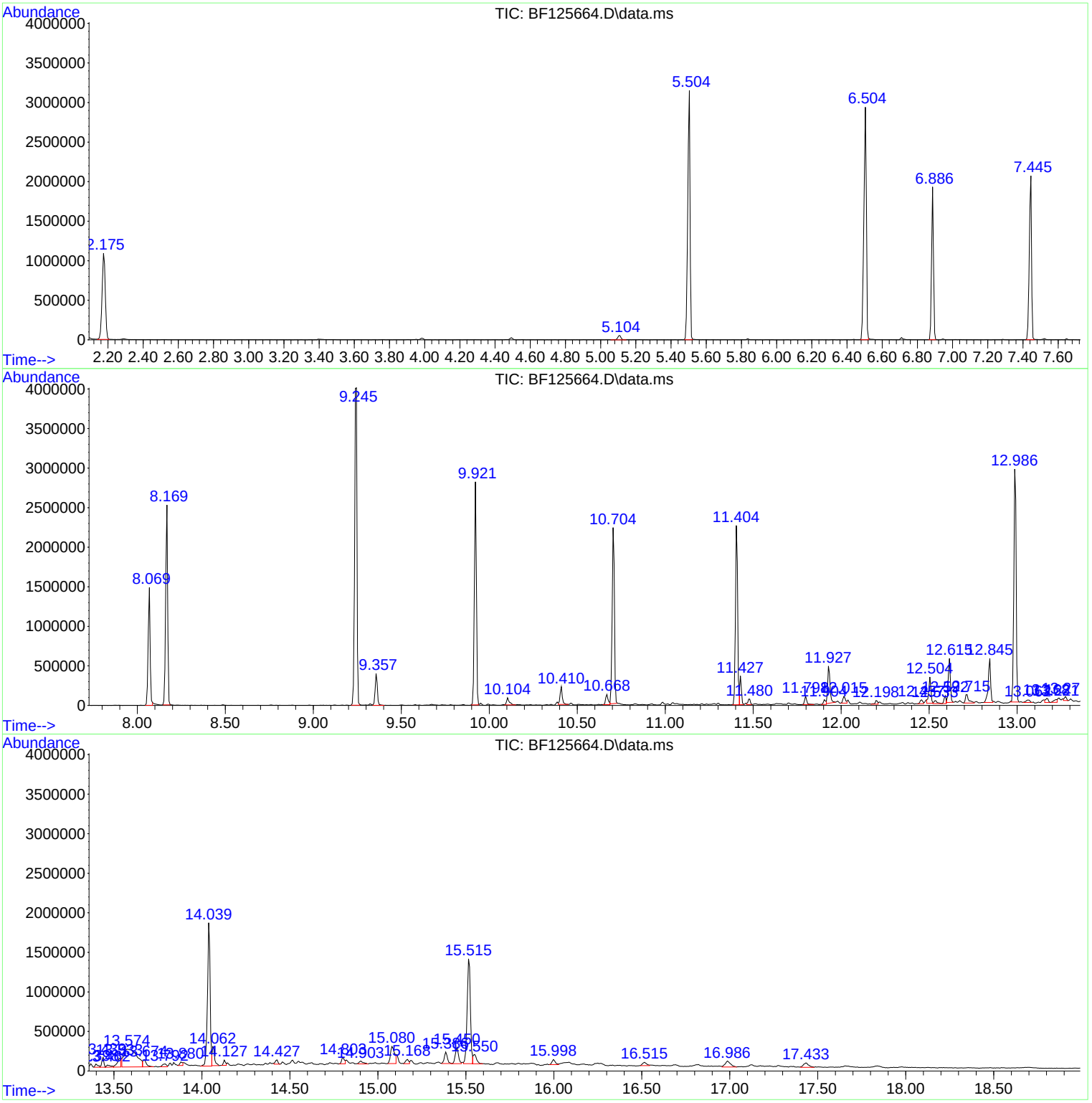
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-DB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.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\BF092521\
Data File : BF125664.D
Acq On : 25 Sep 2021 19:08
Operator : JU/CG
Sample : M3943-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-DB-1

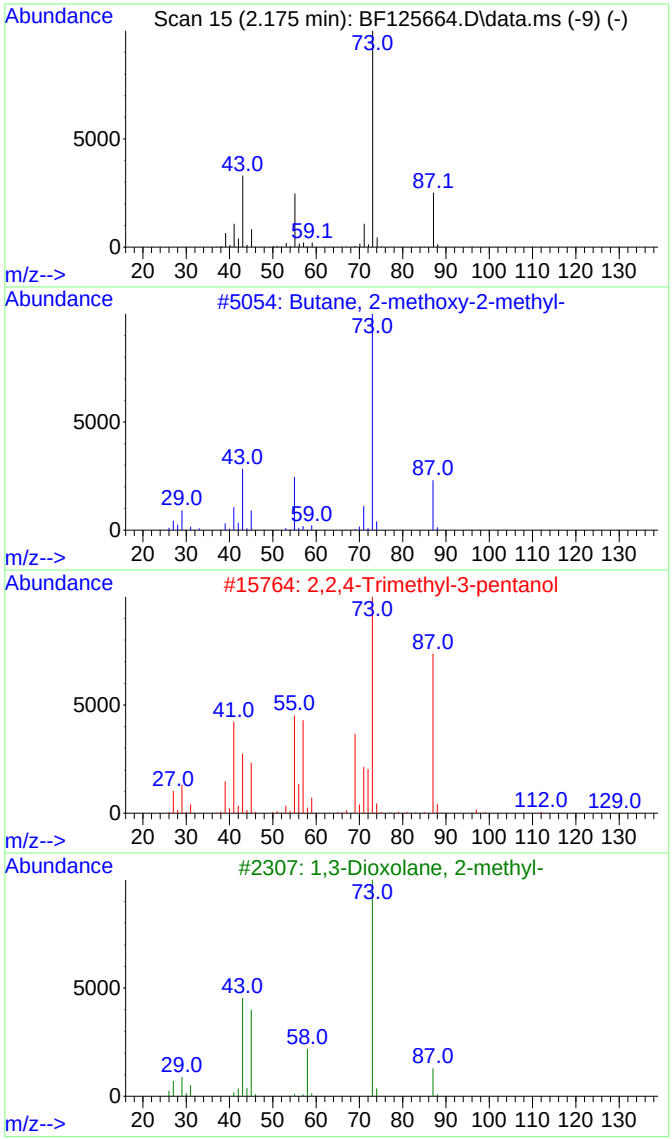
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

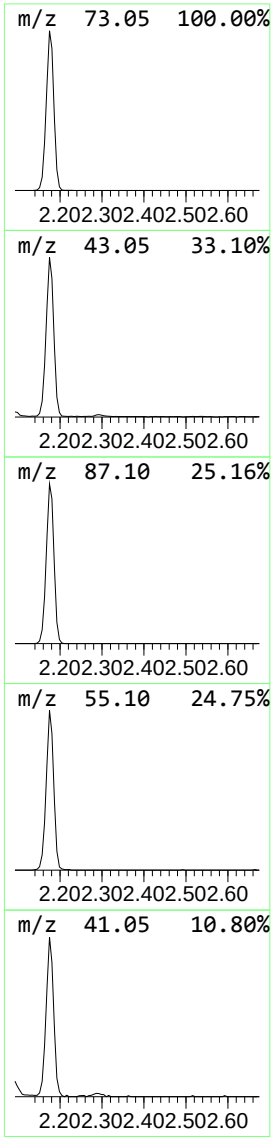
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	18.71 ng	1371220	1,4-Dichlorobenzene-d4	6.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092521\
Data File : BF125664.D
Acq On : 25 Sep 2021 19:08
Operator : JU/CG
Sample : M3943-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-DB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

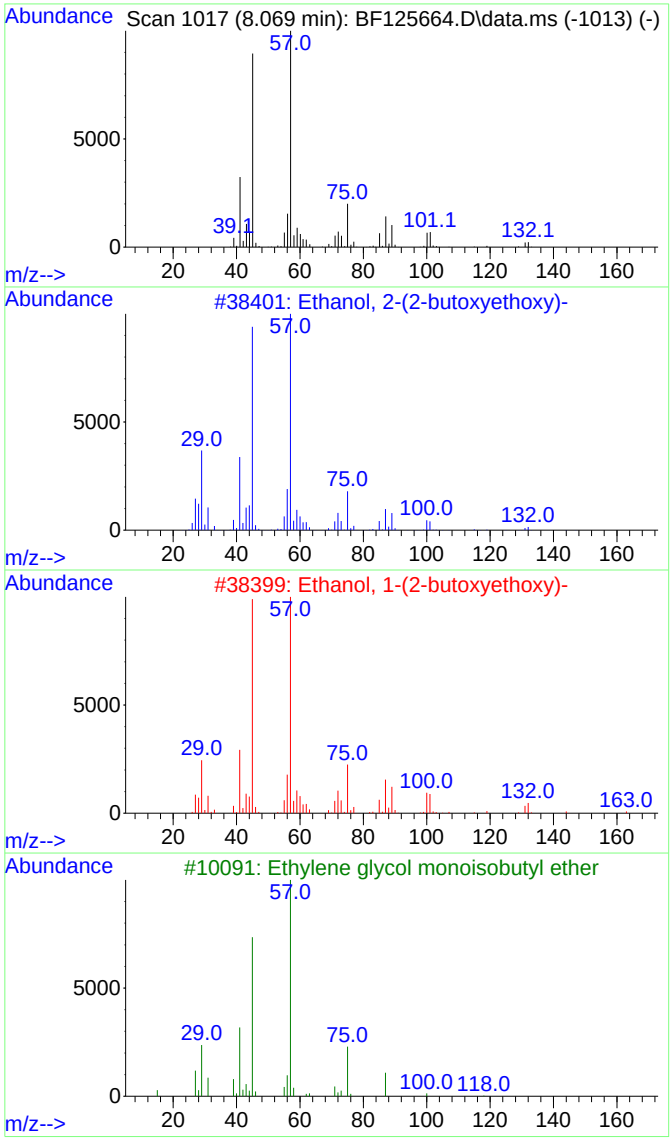
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

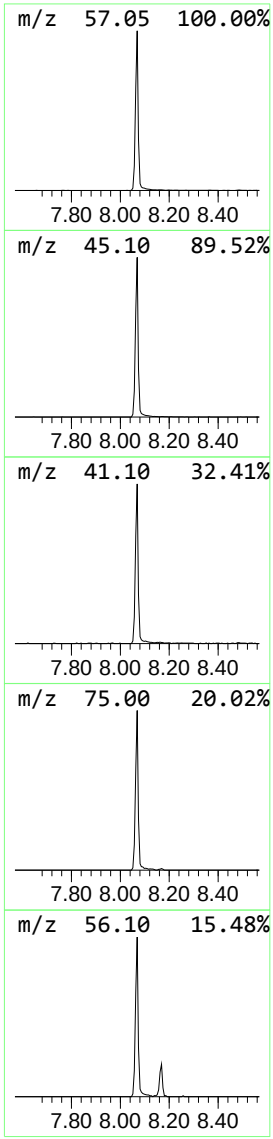
****

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.069	11.65 ng	1160660	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092521\
Data File : BF125664.D
Acq On : 25 Sep 2021 19:08
Operator : JU/CG
Sample : M3943-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-DB-1

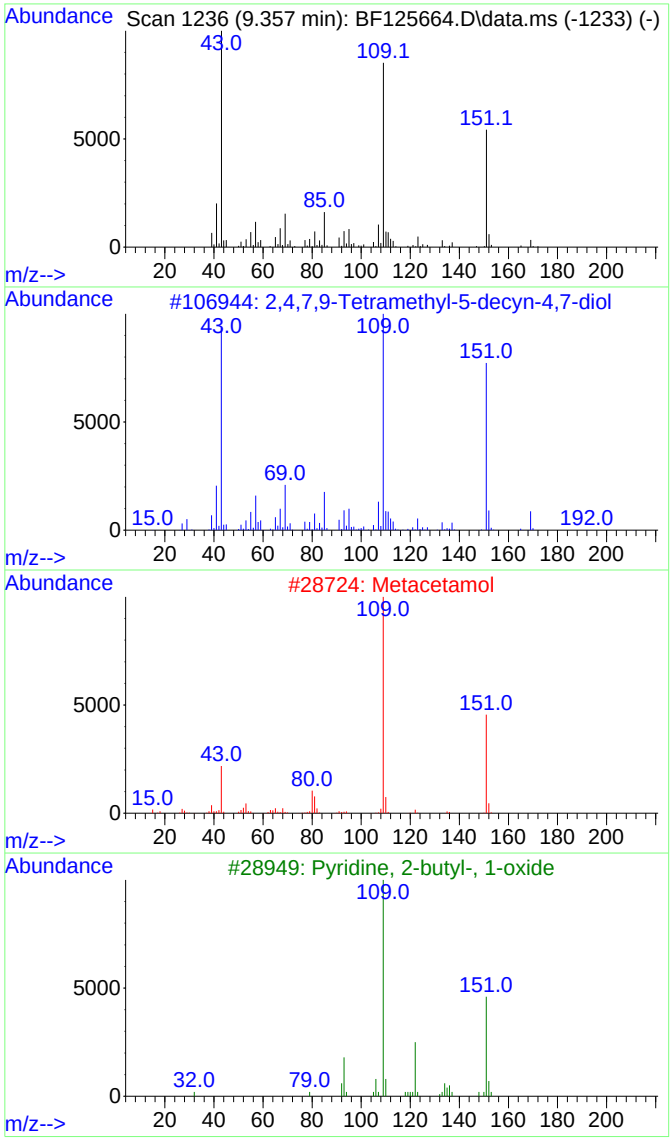
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

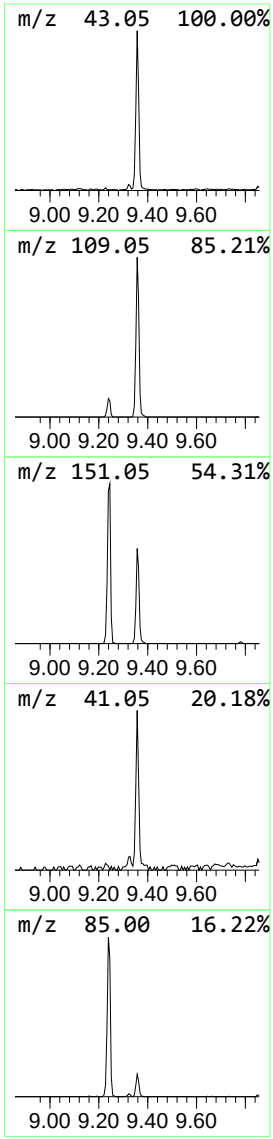
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.357	3.12 ng	348276	Acenaphthene-d10	9.921

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	Metacetamol	151	C8H9NO2	000621-42-1	64
3	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092521\
Data File : BF125664.D
Acq On : 25 Sep 2021 19:08
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Sample : M3943-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-DB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

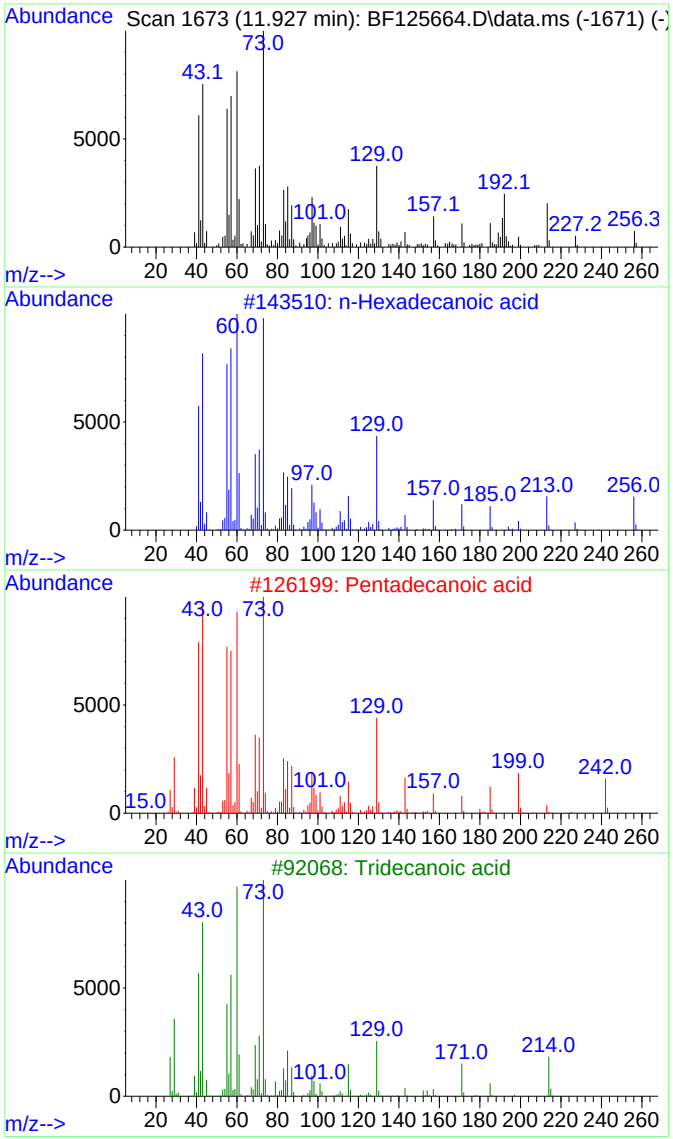
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

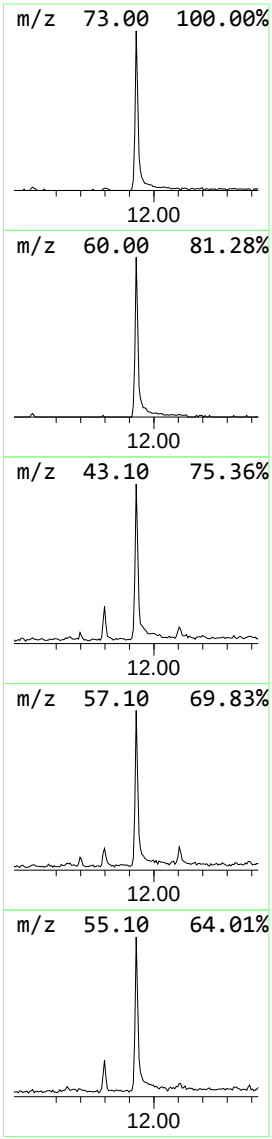
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	4.26 ng	426342	Phenanthrene-d10	11.404

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	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Dodecanoic acid	200	C12H24O2	000143-07-7	62





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Sample : M3943-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-DB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

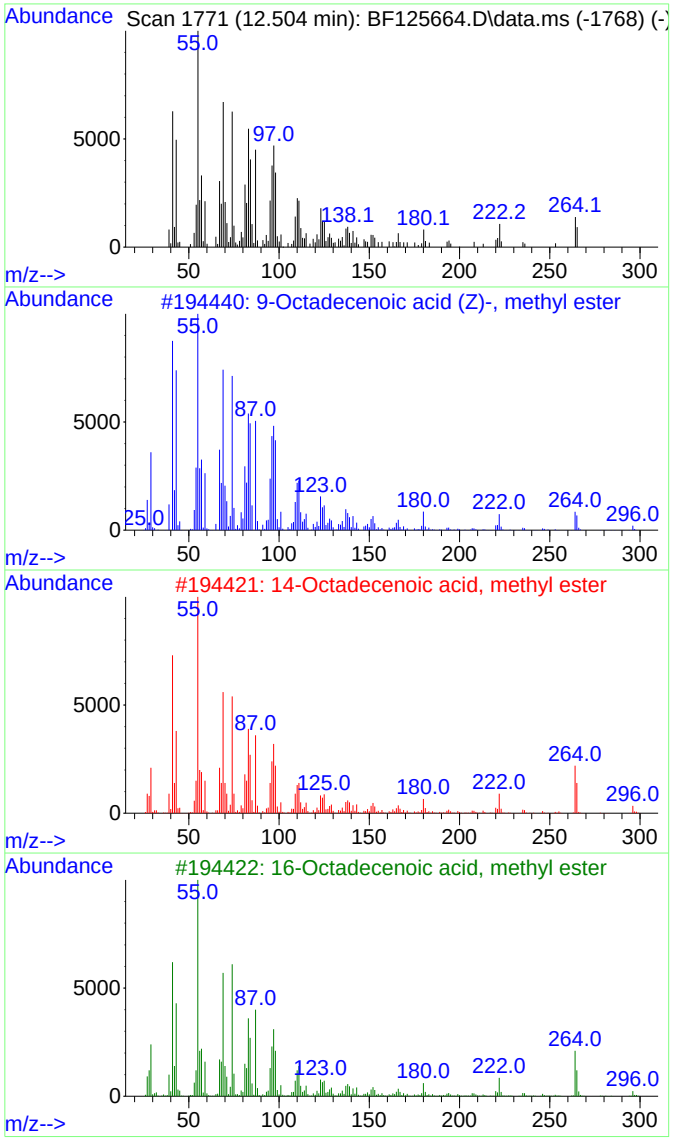
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

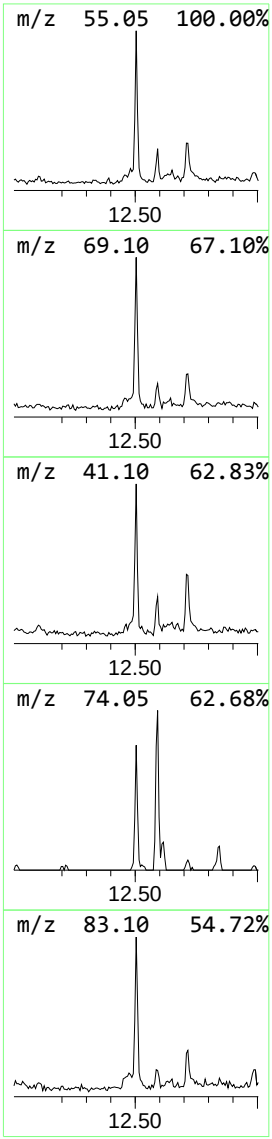
****

Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.504	2.72 ng	272261	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	91
4	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	91
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	91





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Data File : BF125664.D
Acq On : 25 Sep 2021 19:08
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Sample : M3943-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-DB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

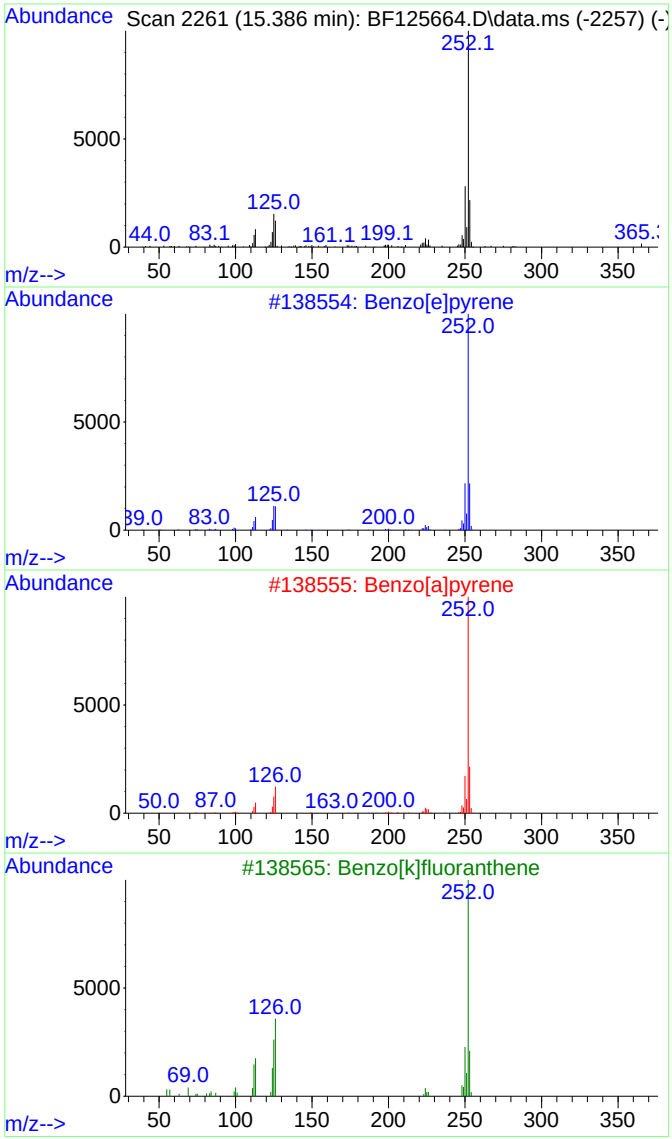
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

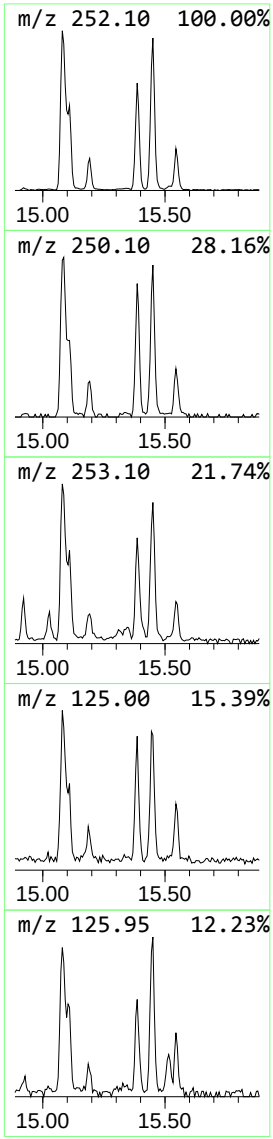
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.386	2.06 ng	177226	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092521\
Data File : BF125664.D
Acq On : 25 Sep 2021 19:08
Operator : JU/CG
Sample : M3943-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-DB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.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
Butane, 2-metho...	2.175	18.7	ng	1371220	1	6.886	1465960	20.0
Ethanol, 2-(2-b...	8.069	11.7	ng	1160660	2	8.169	1991860	20.0
2,4,7,9-Tetrame...	9.357	3.1	ng	348276	3	9.921	2233710	20.0
n-Hexadecanoic ...	11.927	4.3	ng	426342	4	11.404	2001760	20.0
9-Octadecenoic ...	12.504	2.7	ng	272261	4	11.404	2001760	20.0
Benzo[e]pyrene	15.386	2.1	ng	177226	6	15.515	1718690	20.0