LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010821\
Data File : BF122947.D
Acq On : 8 Jan 2021 18:32
Operator : JU/CG
Sample : M1044-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4

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-BF010721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122947.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	19	25	33	rVB	522692	723919	16.15%	1.846%
2	2.340	39	43	49	rVB	61289	85732	1.91%	0.219%
3	3.428	225	228	234	rBV	38261	71888	1.60%	0.183%
4	4.034	327	331	337	rVB	58554	73470	1.64%	0.187%
5	5.140	515	519	525	rVB	331987	398014	8.88%	1.015%
6	5.534	580	586	589	rBV	4280604	4151837	92.61%	10.589%
7	5.934	651	654	660	rVB	54183	51373	1.15%	0.131%
8	6.534	750	756	759	rBV	3960808	4127132	92.06%	10.526%
9	6.734	788	790	796	rVB3	82517	110412	2.46%	0.282%
10	6.916	817	821	824	rBV	1323072	1000338	22.31%	2.551%
11	7.475	906	916	919	rBV	2881214	2583842	57.63%	6.590%
12	8.198	1034	1039	1042	rBV	1561179	1320524	29.45%	3.368%
13	9.275	1217	1222	1226	rBV	4910503	4483262	100.00%	11.434%
14	9.363	1232	1237	1240	rBV4	71138	101192	2.26%	0.258%
15	9.392	1240	1242	1245	rVB	75990	62027	1.38%	0.158%
16	9.669	1286	1289	1293	rVB	254555	225270	5.02%	0.575%
17	9.957	1330	1338	1341	rBV	1733637	1422791	31.74%	3.629%
18	9.992	1341	1344	1347	rVB2	55263	53298	1.19%	0.136%
19	10.369	1404	1408	1410	rBV	113803	101663	2.27%	0.259%
20	10.504	1428	1431	1435	rBV3	47182	52265	1.17%	0.133%
21	10.745	1467	1472	1475	rBV	3188267	2726017	60.80%	6.952%
22	10.869	1490	1493	1500	rVB4	51604	79322	1.77%	0.202%
23	11.316	1562	1569	1572	rBV5	39348	75869	1.69%	0.193%
24	11.445	1588	1591	1594	rBV	1416923	1349678	30.10%	3.442%
25	11.469	1594	1595	1598	rVV	492519	344906	7.69%	0.880%
26	11.522	1602	1604	1607	rVB	137734	102737	2.29%	0.262%
27	11.951	1674	1677	1679	rBV	99903	98006	2.19%	0.250%
28	11.975	1679	1681	1686	rVB2	414574	371855	8.29%	0.948%
29	12.063	1692	1696	1699	rBV	153190	182750	4.08%	0.466%
30	12.245	1724	1727	1729	rBV	67791	60040	1.34%	0.153%
31	12.269	1729	1731	1736	rVB2	40312	64173	1.43%	0.164%
32	12.398	1751	1753	1756	rBV2	55820	46845	1.04%	0.119%
33	12.439	1756	1760	1765	rBV2	212173	230474	5.14%	0.588%
34	12.498	1767	1770	1774	rVV2	107809	135969	3.03%	0.347%
35	12.539	1774	1777	1780	rVV3	72554	102898	2.30%	0.262%
36	12.586	1782	1785	1790	rVB3	59161	74267	1.66%	0.189%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010821\
Data File : BF122947.D
Acq On : 8 Jan 2021 18:32
Operator : JU/CG
Sample : M1044-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4

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-BF010721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.663	1795	1798	1802	rBV	918517	798035	17.80%	2.035%
38	12.763	1812	1815	1817	rBV	85569	80591	1.80%	0.206%
39	12.892	1832	1837	1844	rBV	789038	926218	20.66%	2.362%
40	13.039	1858	1862	1866	rVB	4009623	3935832	87.79%	10.038%
41	13.110	1872	1874	1878	rBV	50985	56658	1.26%	0.145%
42	13.198	1887	1889	1891	rBV2	47146	53395	1.19%	0.136%
43	13.221	1891	1893	1896	rVB	132878	122986	2.74%	0.314%
44	13.292	1902	1905	1907	rVB	82725	70891	1.58%	0.181%
45	13.327	1908	1911	1914	rVB2	111714	104058	2.32%	0.265%
46	13.451	1930	1932	1934	rBV	61380	50738	1.13%	0.129%
47	13.939	2012	2015	2020	rBV	751985	689185	15.37%	1.758%
48	14.098	2037	2042	2044	rBV2	1456643	1699172	37.90%	4.334%
49	14.121	2044	2046	2049	rVB	405655	302962	6.76%	0.773%
50	14.739	2148	2151	2154	rBV	300398	278855	6.22%	0.711%
51	15.151	2217	2221	2224	rBV	366291	562553	12.55%	1.435%
52	15.463	2271	2274	2280	rVB	241991	293969	6.56%	0.750%
53	15.521	2281	2284	2290	rVB	378049	438370	9.78%	1.118%
54	15.592	2292	2296	2299	rBV	1009719	1151124	25.68%	2.936%
55	17.092	2547	2551	2559	rVB2	175850	347708	7.76%	0.887%

Sum of corrected areas: 39209355

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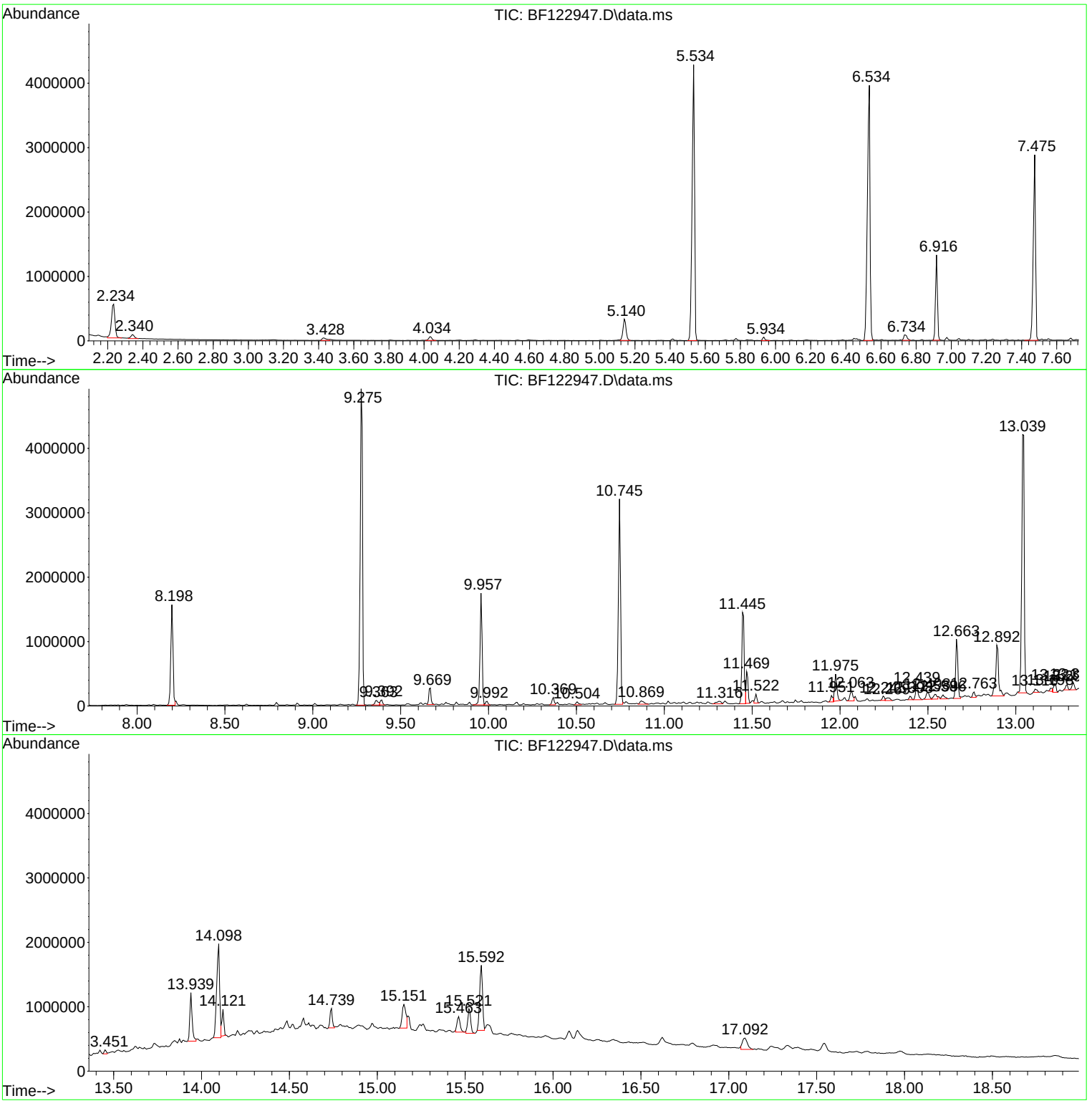
Data File : BF122947.D
Acq On : 8 Jan 2021 18:32
Operator : JU/CG
Sample : M1044-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.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\BF010821\
Data File : BF122947.D
Acq On : 8 Jan 2021 18:32
Operator : JU/CG
Sample : M1044-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

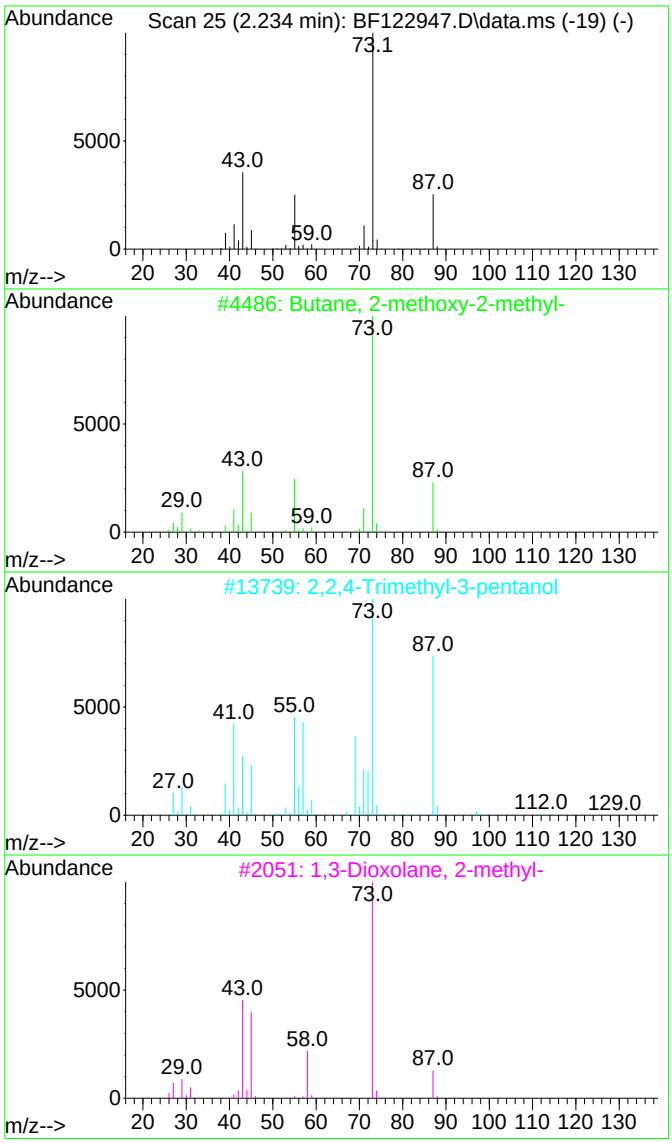
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

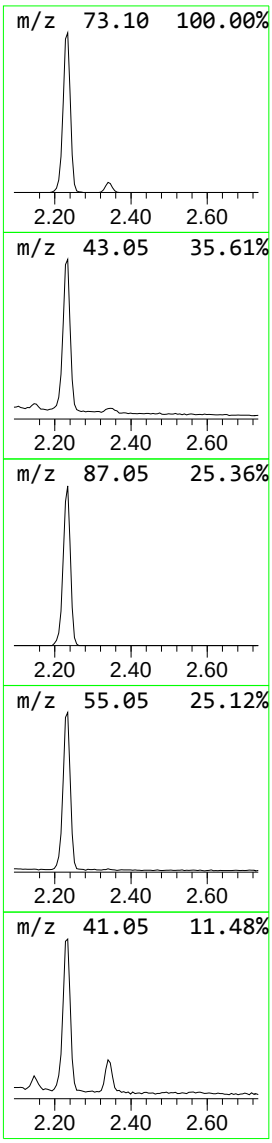
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.234	14.47 ng	723919	1,4-Dichlorobenzene-d4	6.916

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	25
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\BF010821\
Data File : BF122947.D
Acq On : 8 Jan 2021 18:32
Operator : JU/CG
Sample : M1044-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

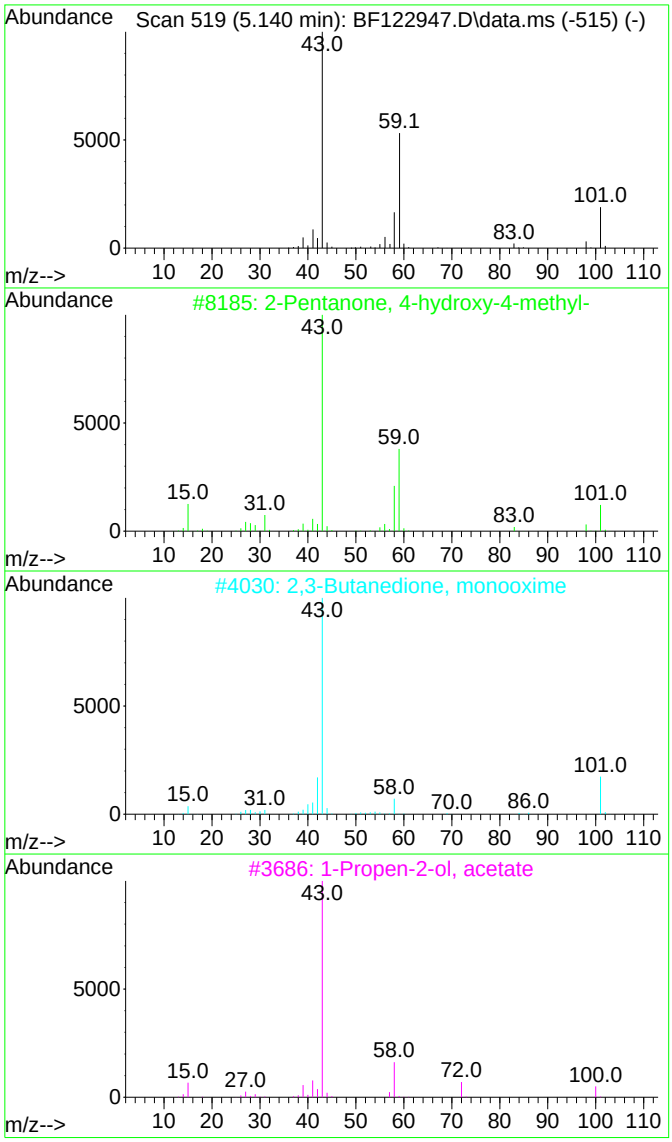
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

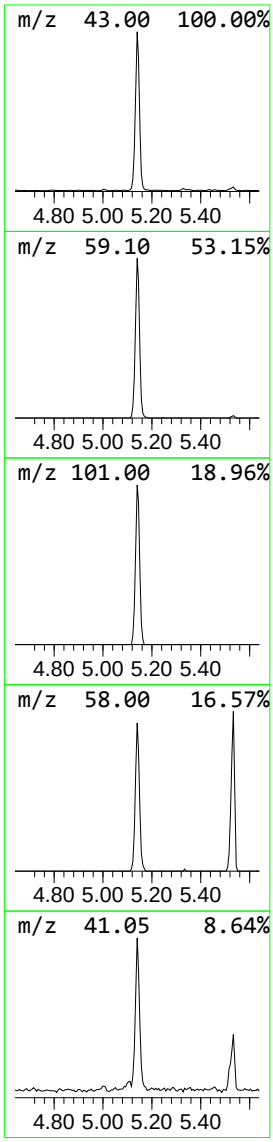
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.140	7.96 ng	398014	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010821\
Data File : BF122947.D
Acq On : 8 Jan 2021 18:32
Operator : JU/CG
Sample : M1044-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4

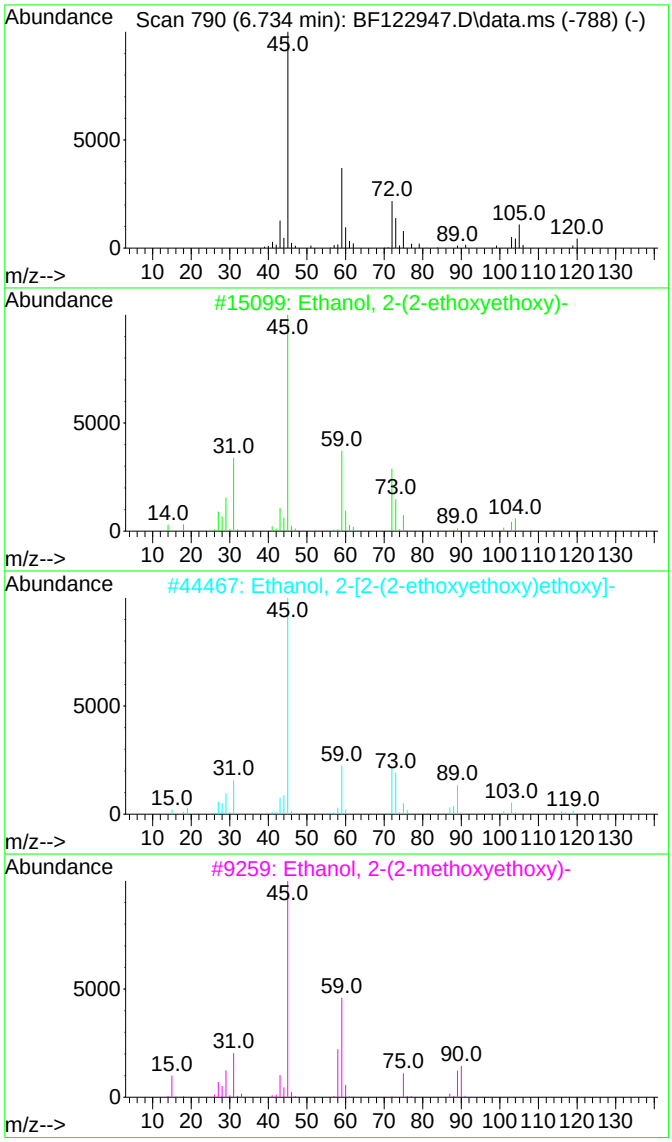
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

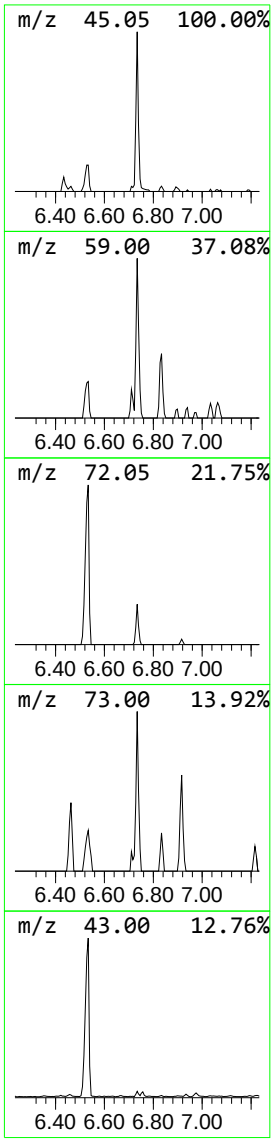
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.734	2.21 ng	110412	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	86
2	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	59
3	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	40
4	Methyl 2-(2-methoxyethoxy)acetate	148	C6H12O4	1000366-88-1	36
5	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010821\
Data File : BF122947.D
Acq On : 8 Jan 2021 18:32
Operator : JU/CG
Sample : M1044-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

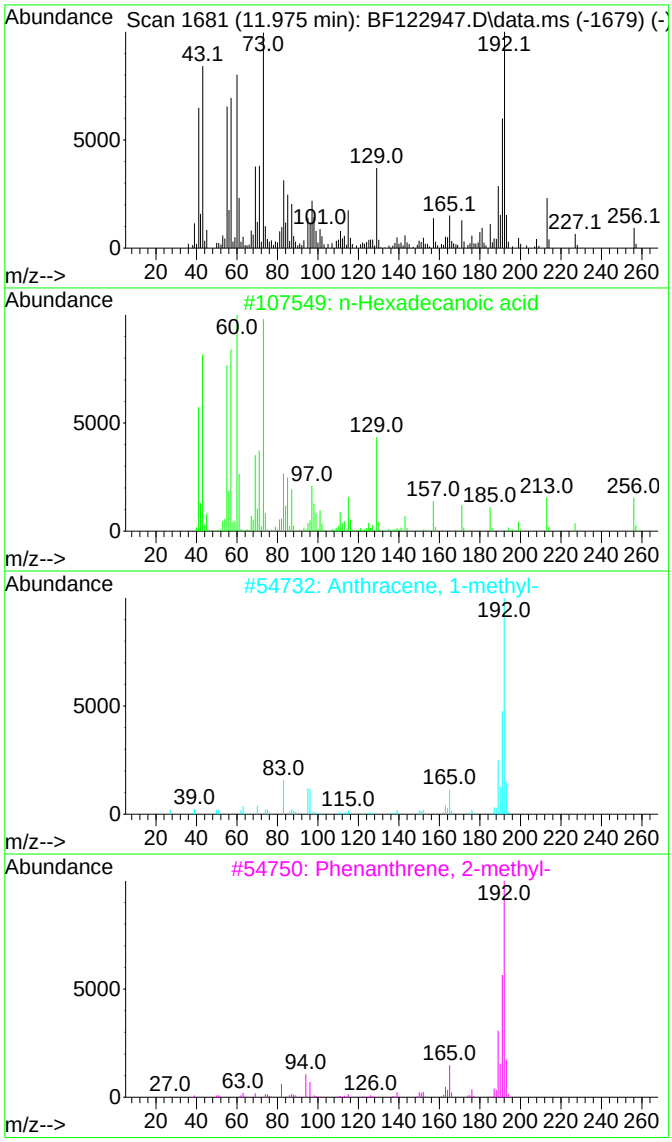
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

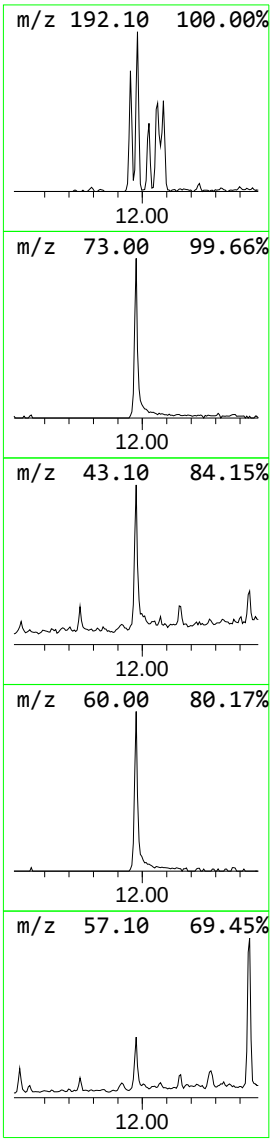
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.975	5.51 ng	371855	Phenanthrene-d10	11.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	92
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	92
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	92
5	Tridecanoic acid	214	C13H26O2	000638-53-9	89





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010821\
Data File : BF122947.D
Acq On : 8 Jan 2021 18:32
Operator : JU/CG
Sample : M1044-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

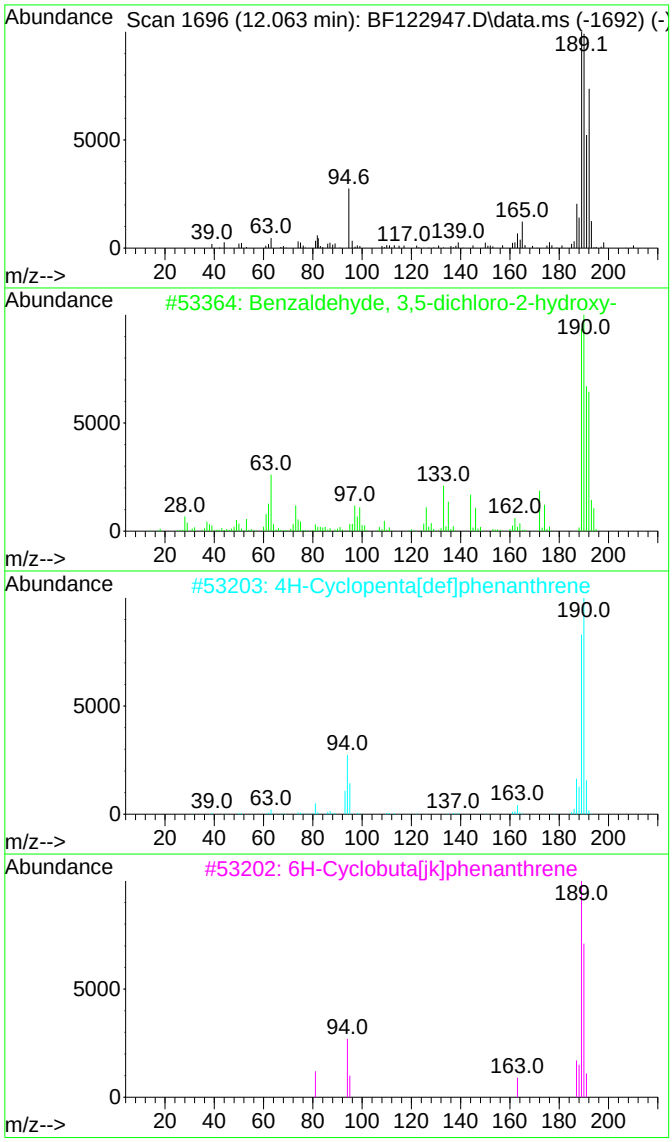
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

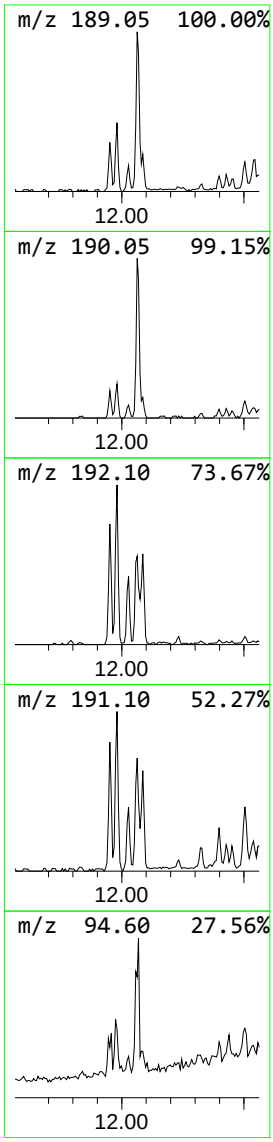
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzaldehyde, 3,5-dichloro-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.063	2.71 ng	182750	Phenanthrene-d10	11.445

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	60
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	47
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	38
5	3-Bromo-2-furoic acid	190	C5H3BrO3	014903-90-3	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010821\
Data File : BF122947.D
Acq On : 8 Jan 2021 18:32
Operator : JU/CG
Sample : M1044-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

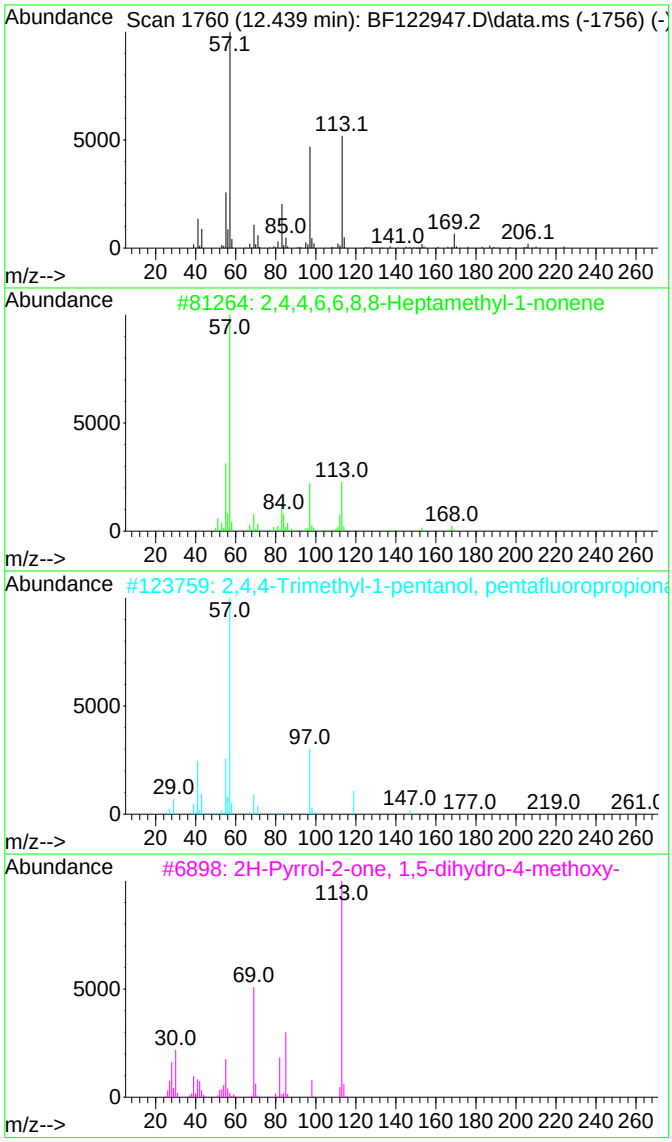
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

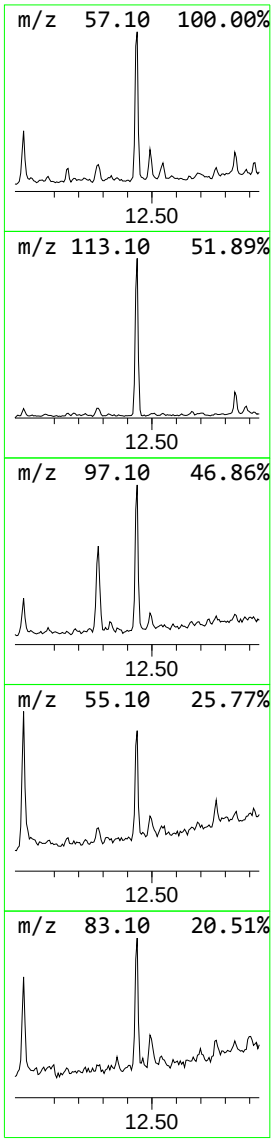
****

Peak Number 6 unknown12.439 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.439	3.42 ng	230474	Phenanthrene-d10	11.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	45
2	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	22
3	2H-Pyrrol-2-one, 1,5-dihydro-4-m...	113	C5H7NO2	069778-83-2	16
4	Pyrrolidine, 1-(6-hydroxy-1-oxoo...	353	C22H43NO2	056666-42-3	16
5	13-Cyclopentyltridecanoic acid, ...	335	C22H41NO	1000336-07-1	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010821\
Data File : BF122947.D
Acq On : 8 Jan 2021 18:32
Operator : JU/CG
Sample : M1044-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

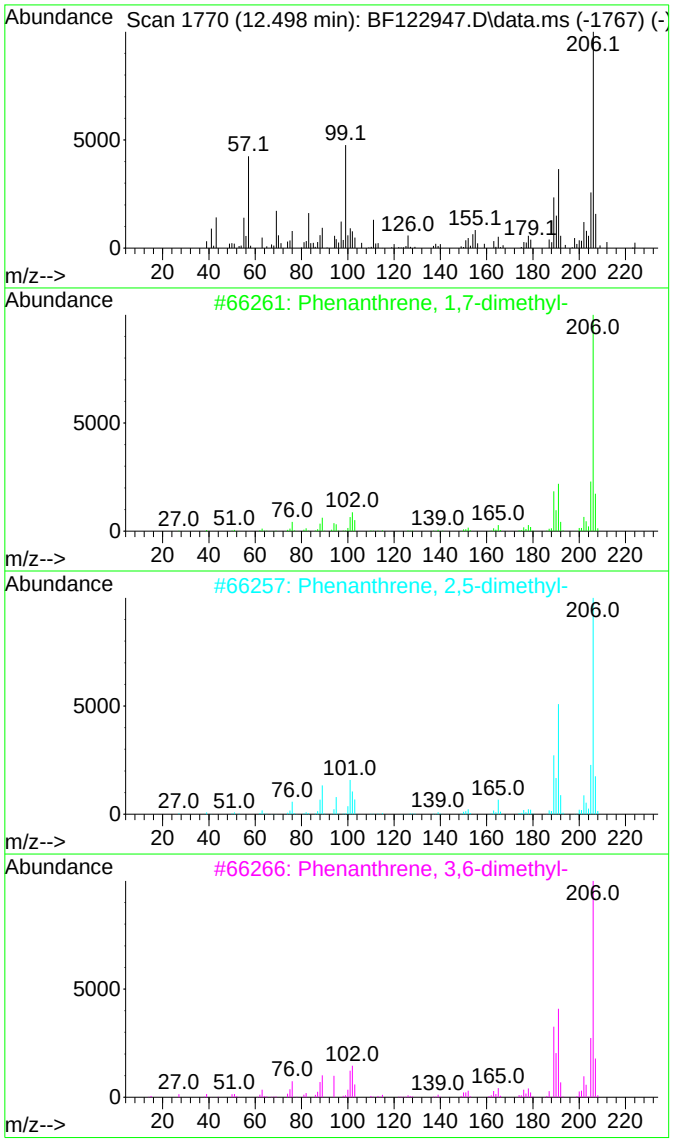
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

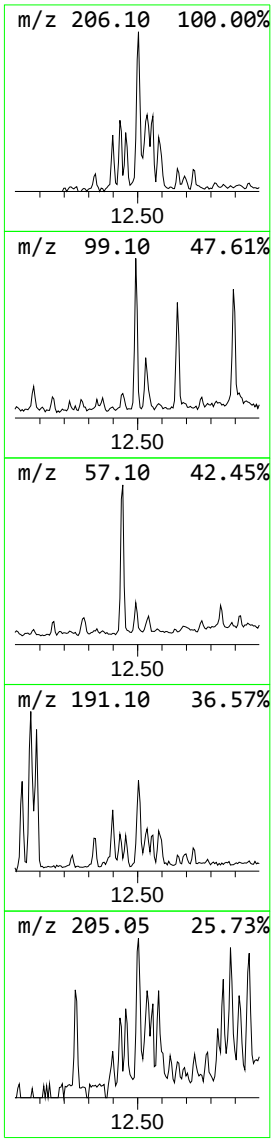
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Phenanthrene, 1,7-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.498	2.01 ng	135969	Phenanthrene-d10	11.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	96
2	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	94
3	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	94
4	di-p-Tolylacetylene	206	C16H14	002789-88-0	90
5	Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	89





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010821\
Data File : BF122947.D
Acq On : 8 Jan 2021 18:32
Operator : JU/CG
Sample : M1044-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

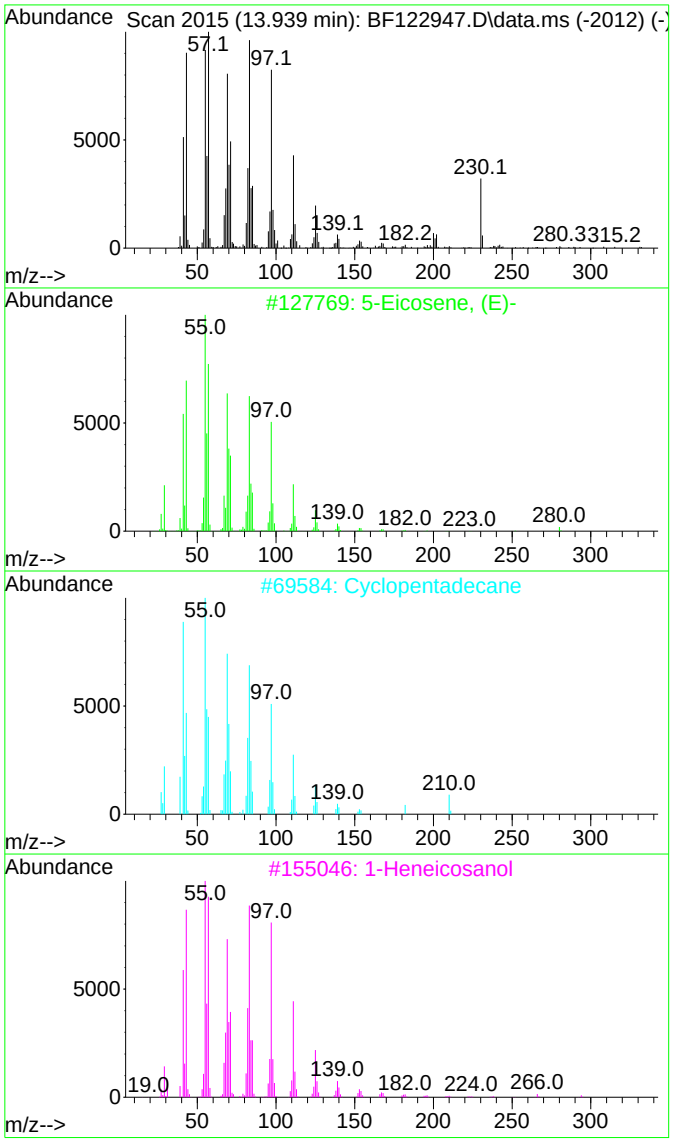
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

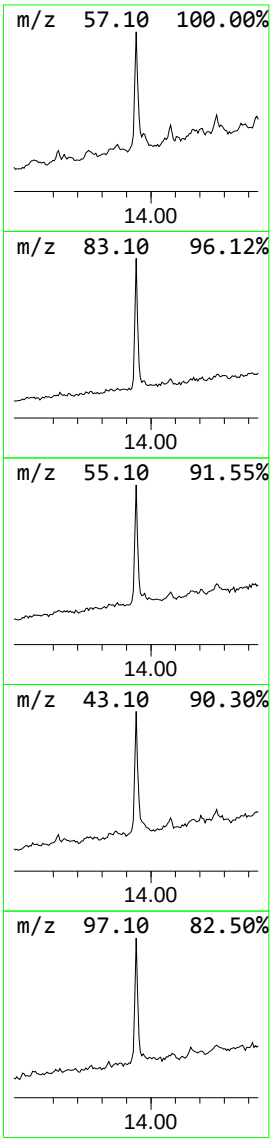
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	8.11 ng	689185	Chrysene-d12	14.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	Cyclopentadecane	210	C15H30	000295-48-7	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	94
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	94





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Acq On : 8 Jan 2021 18:32
Operator : JU/CG
Sample : M1044-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

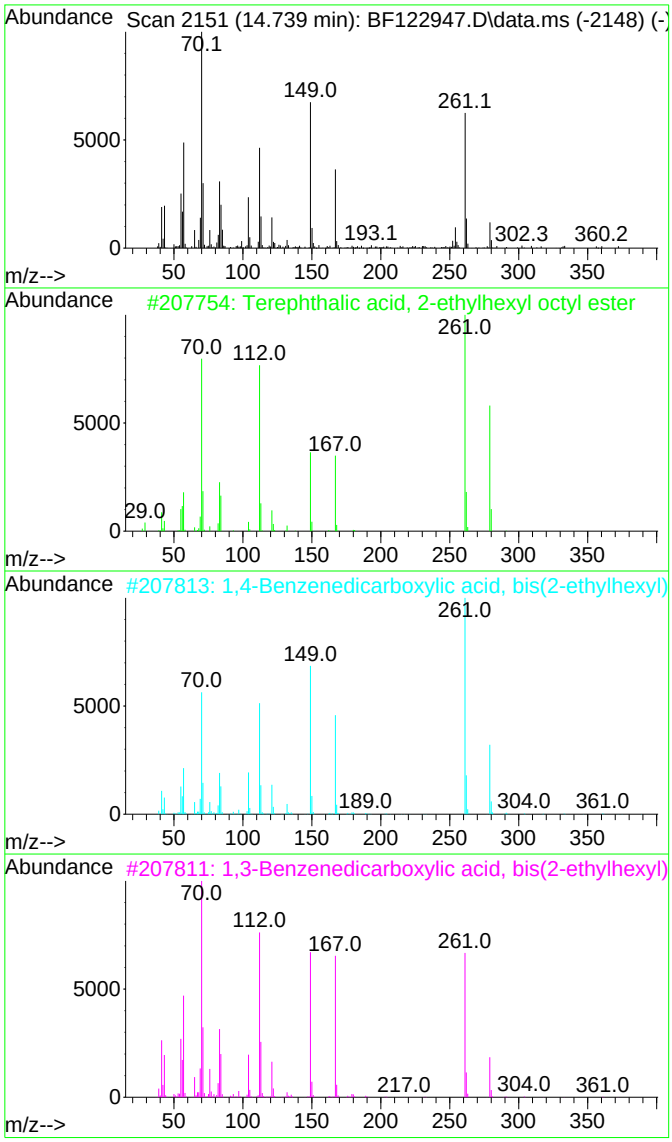
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

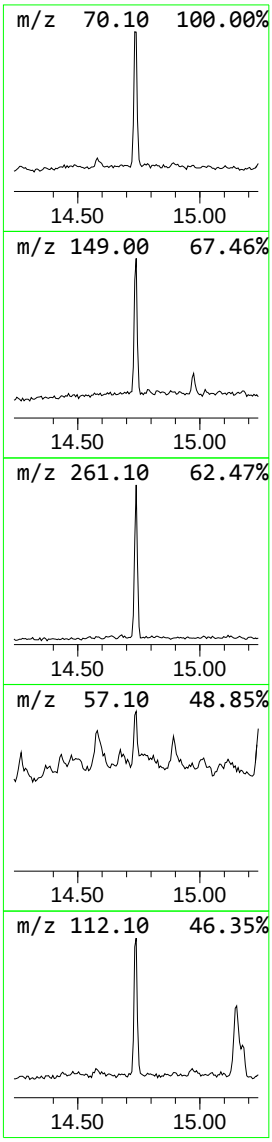
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Terephthalic acid, 2-ethylh... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.739	3.28 ng	278855	Chrysene-d12	14.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	58
2	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	49
3	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	49
4	Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	43
5	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010821\
Data File : BF122947.D
Acq On : 8 Jan 2021 18:32
Operator : JU/CG
Sample : M1044-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

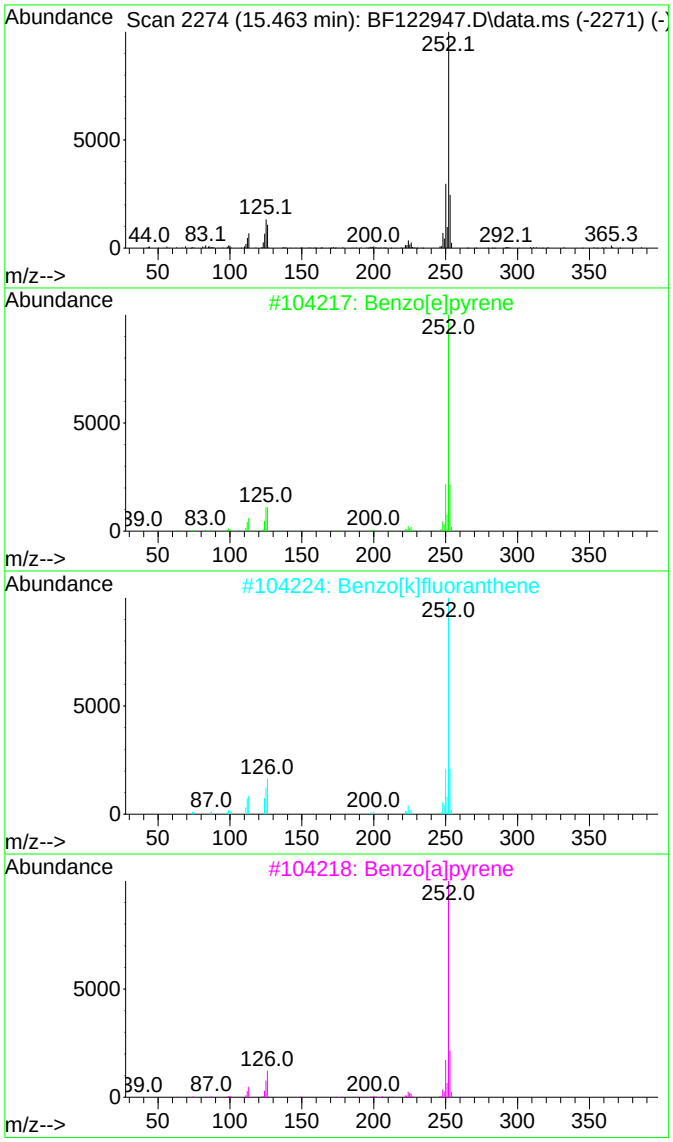
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

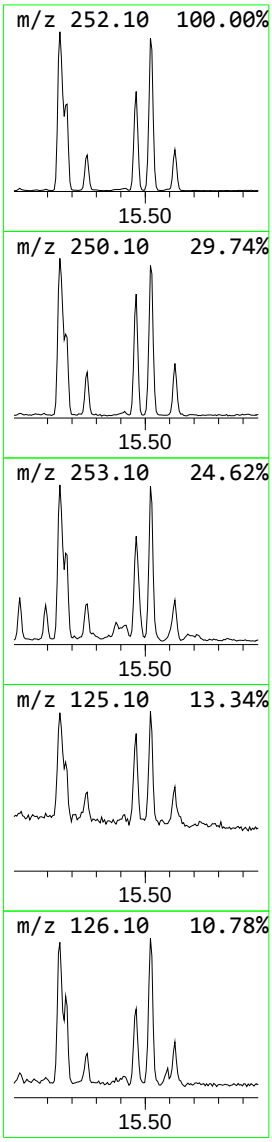
****

Peak Number 10 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.463	5.11 ng	293969	Perylene-d12	15.592

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
3	Benzo[a]pyrene	252	C20H12	000050-32-8	96
4	Perylene	252	C20H12	000198-55-0	95
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010821\
Data File : BF122947.D
Acq On : 8 Jan 2021 18:32
Operator : JU/CG
Sample : M1044-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.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...	2.234	14.5	ng	723919	1	6.916	1000340	20.0
2-Pentanone, 4-...	5.140	8.0	ng	398014	1	6.916	1000340	20.0
Ethanol, 2-(2-e...	6.734	2.2	ng	110412	1	6.916	1000340	20.0
n-Hexadecanoic ...	11.975	5.5	ng	371855	4	11.445	1349680	20.0
Benzaldehyde, 3...	12.063	2.7	ng	182750	4	11.445	1349680	20.0
unknown12.439	12.439	3.4	ng	230474	4	11.445	1349680	20.0
Phenanthrene, 1...	12.498	2.0	ng	135969	4	11.445	1349680	20.0
5-Eicosene, (E)-	13.939	8.1	ng	689185	5	14.098	1699170	20.0
Terephthalic ac...	14.739	3.3	ng	278855	5	14.098	1699170	20.0
Benzo[e]pyrene	15.463	5.1	ng	293969	6	15.592	1151120	20.0