LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010821\
Data File : BF122943.D
Acq On : 8 Jan 2021 16:28
Operator : JU/CG
Sample : M1044-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-12

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: BF122943.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	17	23	28	rVB	428658	576252	16.09%	1.749%
2	2.328	37	41	50	rVB2	50537	77328	2.16%	0.235%
3	3.416	223	226	236	rBV	27728	59727	1.67%	0.181%
4	5.134	510	518	524	rVB	286222	322464	9.00%	0.978%
5	5.528	580	585	588	rBV	3311317	3185258	88.92%	9.665%
6	6.528	750	755	758	rBV	3337162	3294514	91.97%	9.997%
7	6.916	817	821	824	rBV	1237041	954235	26.64%	2.895%
8	7.469	911	915	919	rBV	2068056	2006029	56.00%	6.087%
9	8.198	1035	1039	1042	rBV	1586262	1265394	35.32%	3.840%
10	9.275	1218	1222	1225	rBV	4253782	3558450	99.34%	10.797%
11	9.363	1232	1237	1239	rBV3	51768	66999	1.87%	0.203%
12	9.392	1239	1242	1245	rVB	55455	54522	1.52%	0.165%
13	9.663	1285	1288	1293	rBV	217058	203587	5.68%	0.618%
14	9.957	1334	1338	1341	rBV	1781860	1425014	39.78%	4.324%
15	10.745	1467	1472	1475	rBV	2876301	2421800	67.61%	7.349%
16	10.869	1490	1493	1499	rVB5	40361	59795	1.67%	0.181%
17	11.310	1563	1568	1572	rBV4	91655	117074	3.27%	0.355%
18	11.445	1587	1591	1594	rBV	1606754	1511997	42.21%	4.588%
19	11.469	1594	1595	1598	rVV	451853	309585	8.64%	0.939%
20	11.521	1602	1604	1607	rVB	122672	93459	2.61%	0.284%
21	11.951	1674	1677	1678	rBV	64874	52746	1.47%	0.160%
22	11.974	1678	1681	1685	rVB2	225591	224837	6.28%	0.682%
23	12.063	1693	1696	1698	rBV	97746	106051	2.96%	0.322%
24	12.245	1724	1727	1729	rBV	50758	44243	1.24%	0.134%
25	12.280	1729	1733	1736	rVB2	36774	57982	1.62%	0.176%
26	12.433	1756	1759	1766	rBV	192612	213694	5.97%	0.648%
27	12.498	1767	1770	1773	rVV2	85541	100676	2.81%	0.305%
28	12.539	1774	1777	1782	rVB3	49783	75186	2.10%	0.228%
29	12.663	1795	1798	1801	rBV	757425	602971	16.83%	1.830%
30	12.710	1804	1806	1812	rVB7	37565	47953	1.34%	0.146%
31	12.763	1812	1815	1817	rBV2	50513	52996	1.48%	0.161%
32	12.892	1831	1837	1840	rBV	770171	783161	21.86%	2.376%
33	13.039	1858	1862	1865	rBV	4166160	3582178	100.00%	10.869%
34	13.110	1871	1874	1878	rBV3	47828	74990	2.09%	0.228%
35	13.221	1891	1893	1896	rVB2	89111	76436	2.13%	0.232%
36	13.292	1902	1905	1907	rVB	65719	60012	1.68%	0.182%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010821\
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Operator : JU/CG
Sample : M1044-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-12

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	13.327	1907	1911	1914	rBV2	76816	91301	2.55%	0.277%
38	13.939	2012	2015	2023	rVB3	496846	478932	13.37%	1.453%
39	14.098	2036	2042	2044	rBV2	1468398	1618743	45.19%	4.912%
40	14.121	2044	2046	2049	rVB	297122	219028	6.11%	0.665%
41	14.204	2057	2060	2063	rVB	50837	49002	1.37%	0.149%
42	14.574	2121	2123	2126	rBV2	63317	55837	1.56%	0.169%
43	15.145	2216	2220	2224	rBV	225884	377060	10.53%	1.144%
44	15.457	2269	2273	2279	rVB	169817	214759	6.00%	0.652%
45	15.515	2280	2283	2288	rVB	194369	229317	6.40%	0.696%
46	15.586	2290	2295	2299	rBV	999648	1193273	33.31%	3.621%
47	16.086	2377	2380	2385	rBV	77836	107760	3.01%	0.327%
48	16.615	2466	2470	2475	rBV	75075	126474	3.53%	0.384%
49	17.080	2545	2549	2559	rVB2	100279	206365	5.76%	0.626%
50	17.239	2572	2576	2586	rVB4	47860	113338	3.16%	0.344%
51	17.533	2622	2626	2634	rVB	80866	155462	4.34%	0.472%

Sum of corrected areas: 32956246

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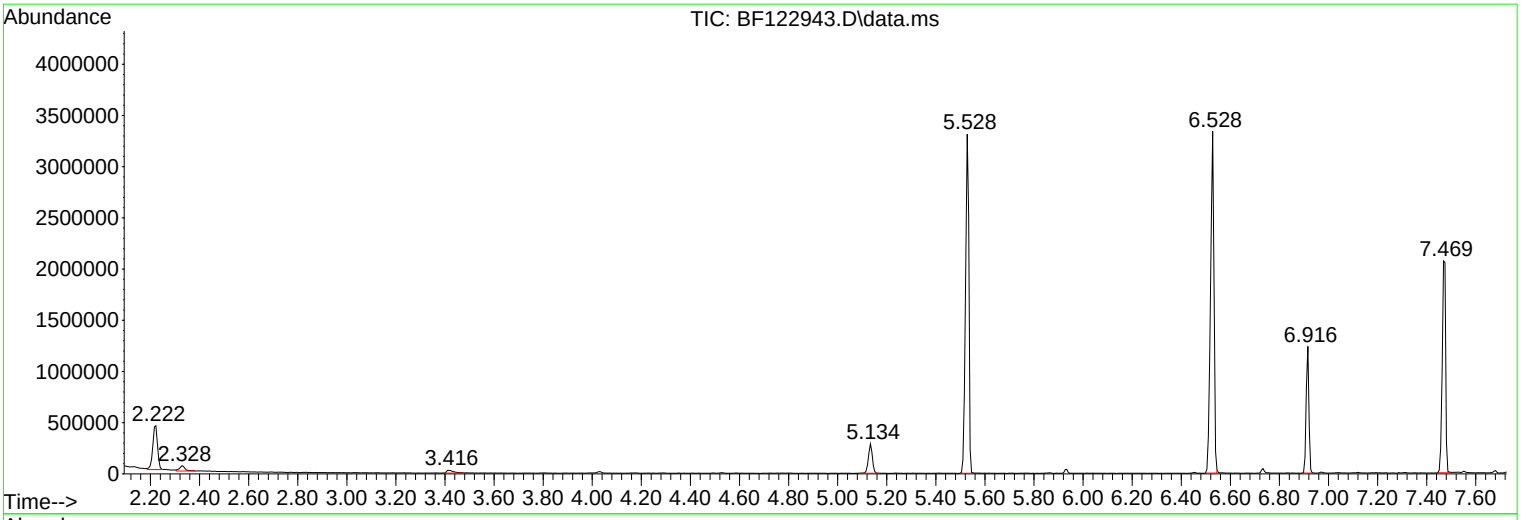
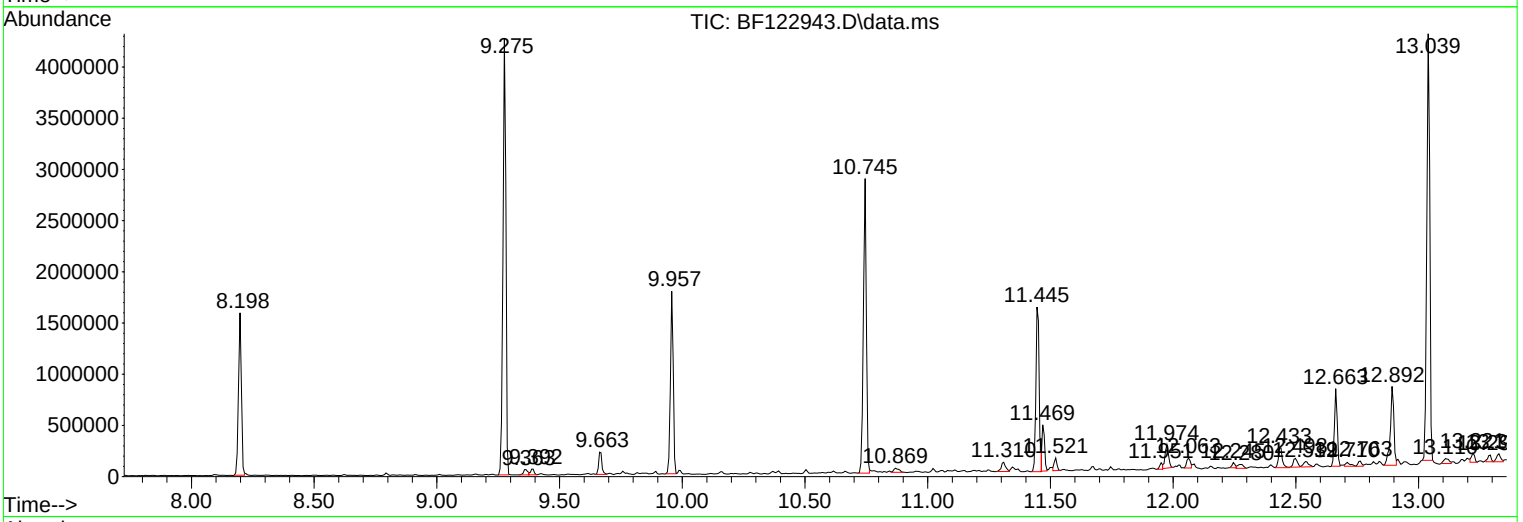
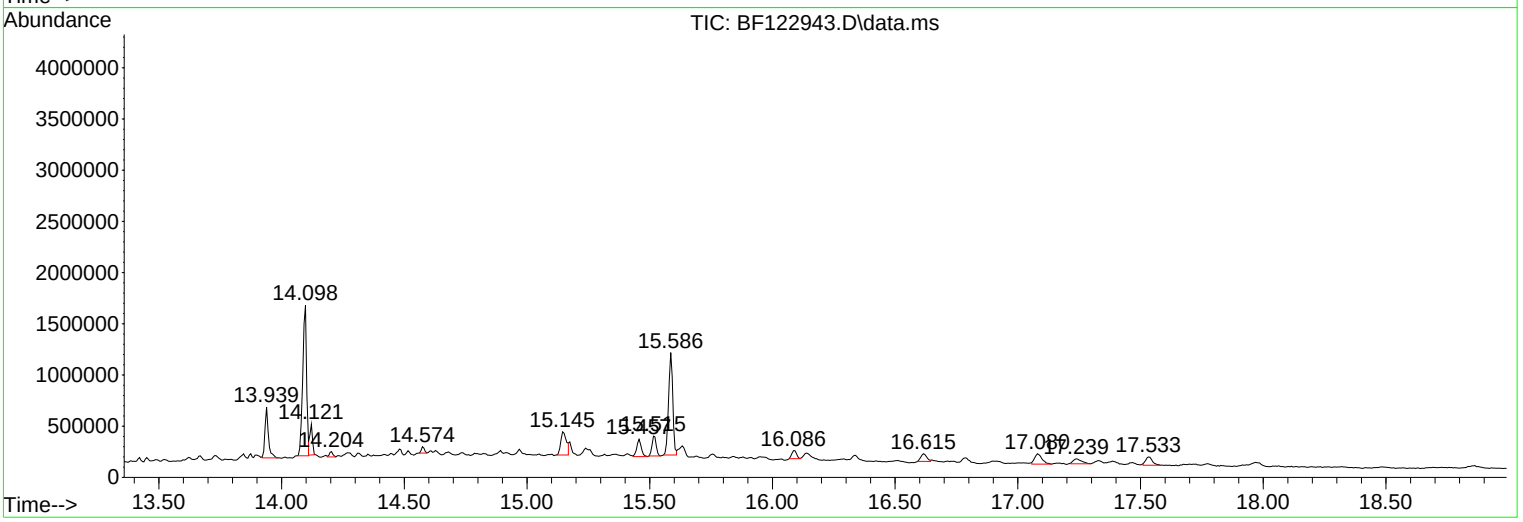
Instrument :
BNA_F
ClientSampleId :
TP-12

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







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Acq On : 8 Jan 2021 16:28
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Sample : M1044-19
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Instrument : BNA_F
ClientSampleId : TP-12

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

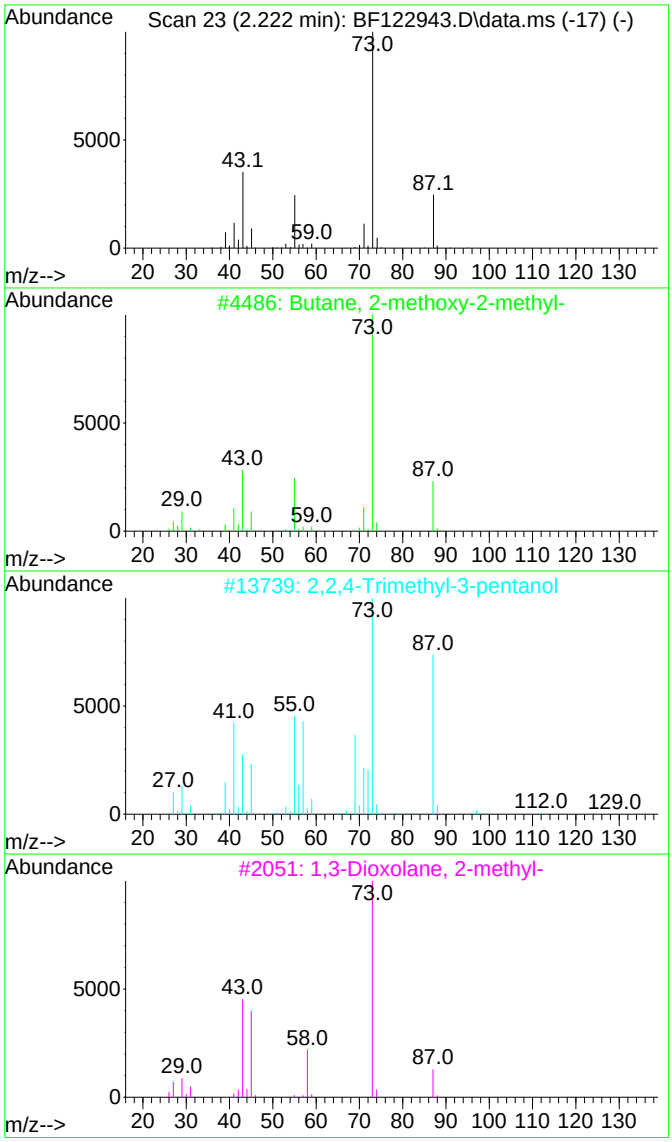
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

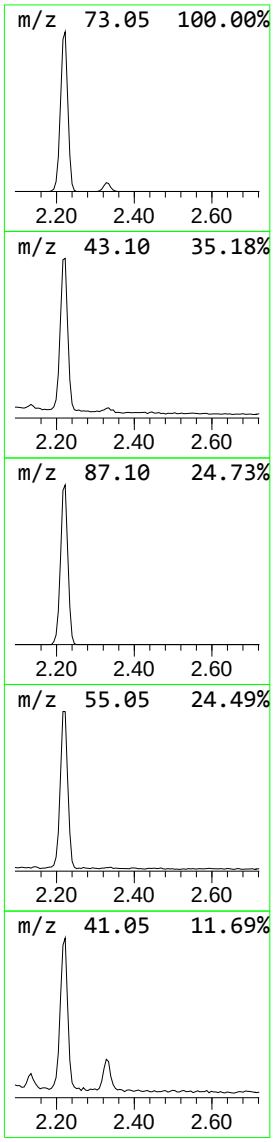
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	12.08 ng	576252	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	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





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Operator : JU/CG
Sample : M1044-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-12

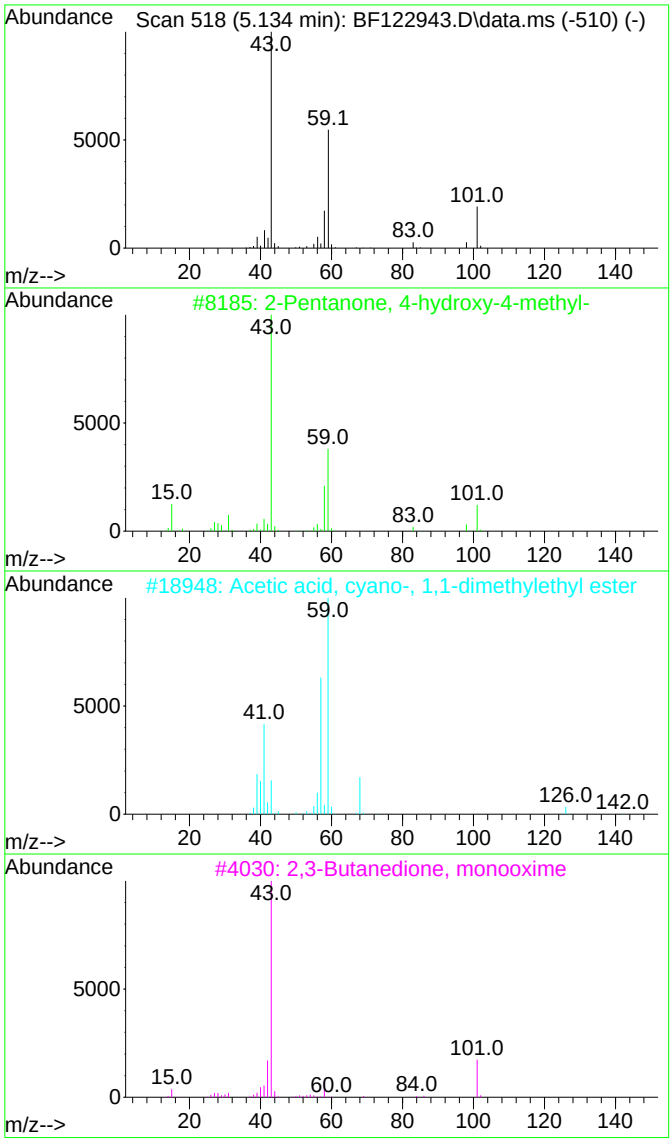
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

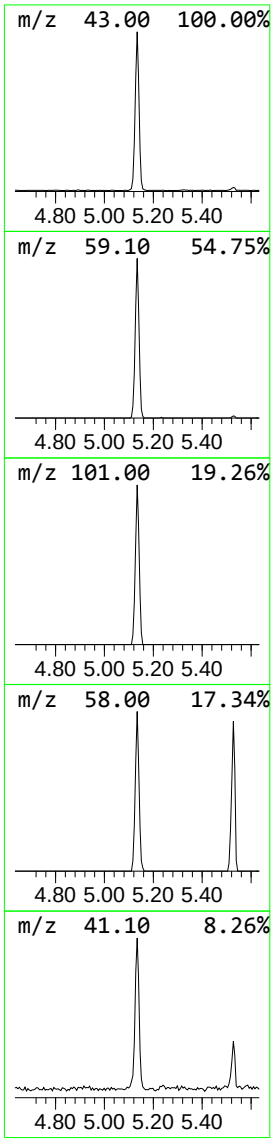
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.134	6.76 ng	322464	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	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





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Data File : BF122943.D
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Operator : JU/CG
Sample : M1044-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-12

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

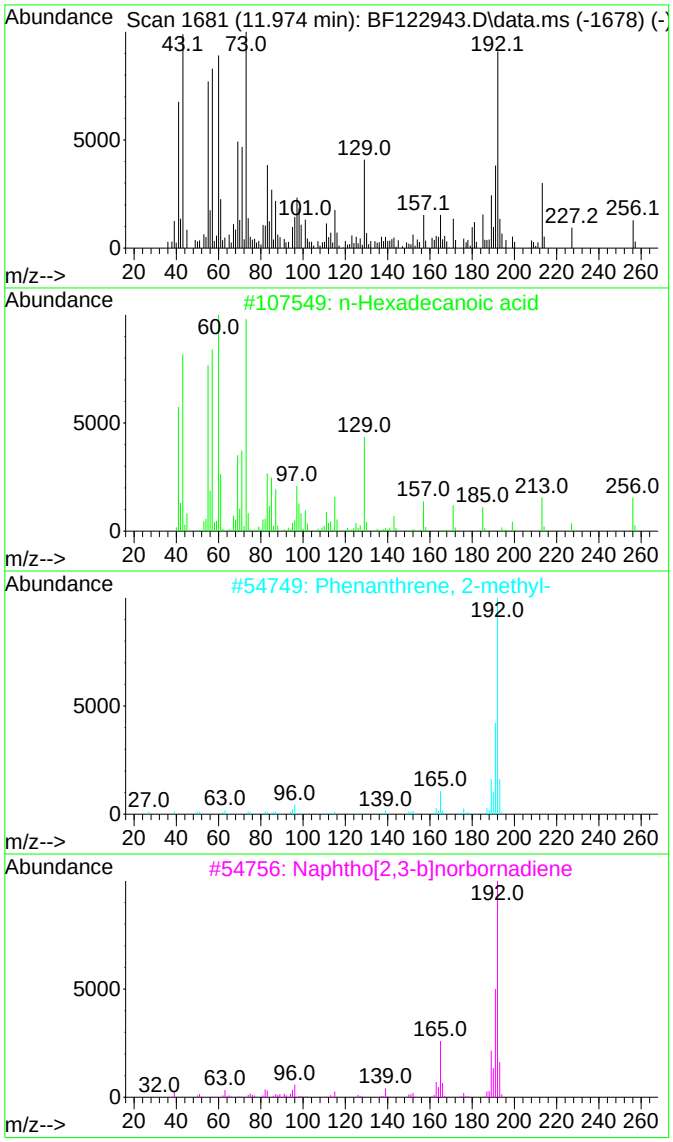
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

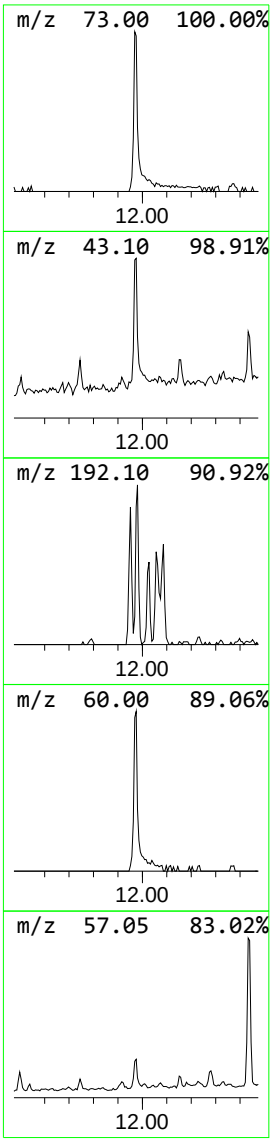
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.974	2.97 ng	224837	Phenanthrene-d10	11.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	66
3	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	64
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	62
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	62





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Sample : M1044-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-12

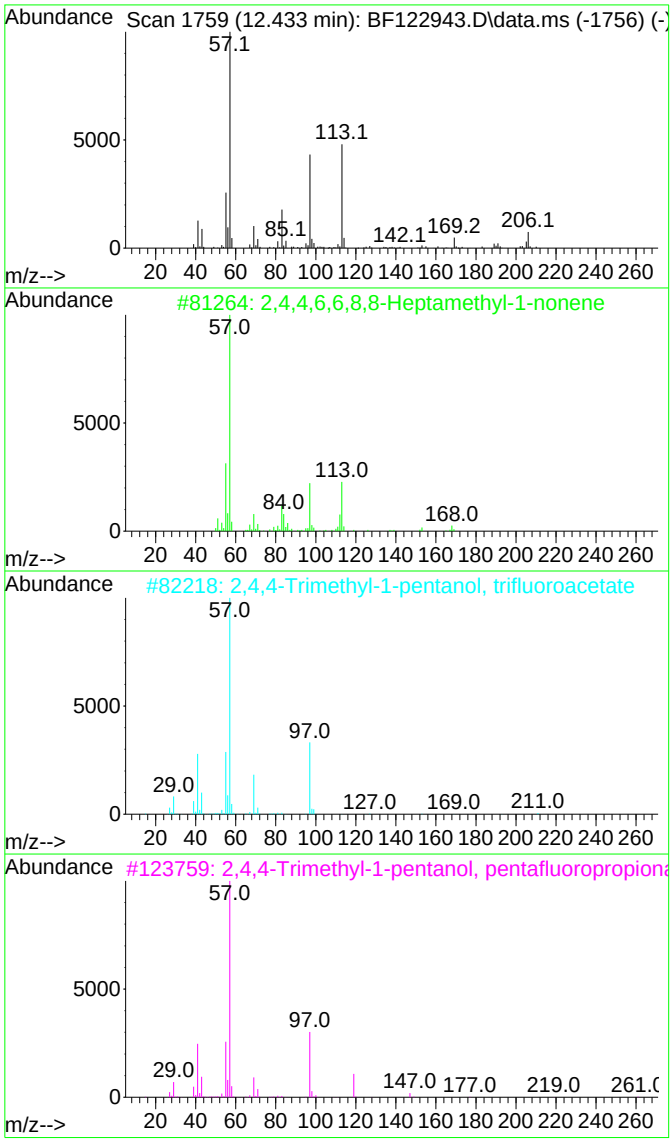
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

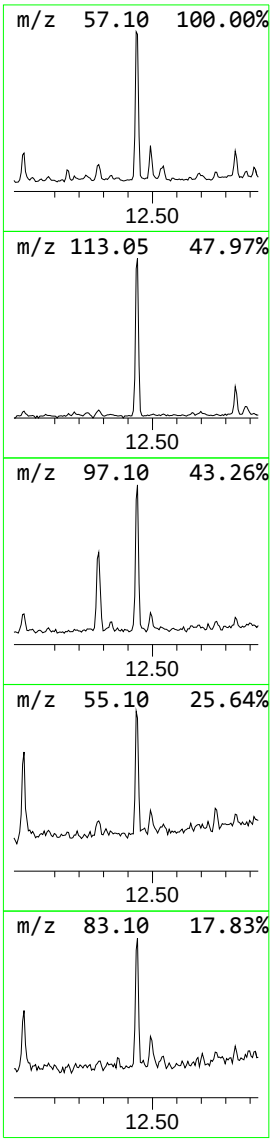
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.433	2.83 ng	213694	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	56
2	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	38
3	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	37
4	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	25
5	Octane, 2-bromo-	192	C8H17Br	000557-35-7	25





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

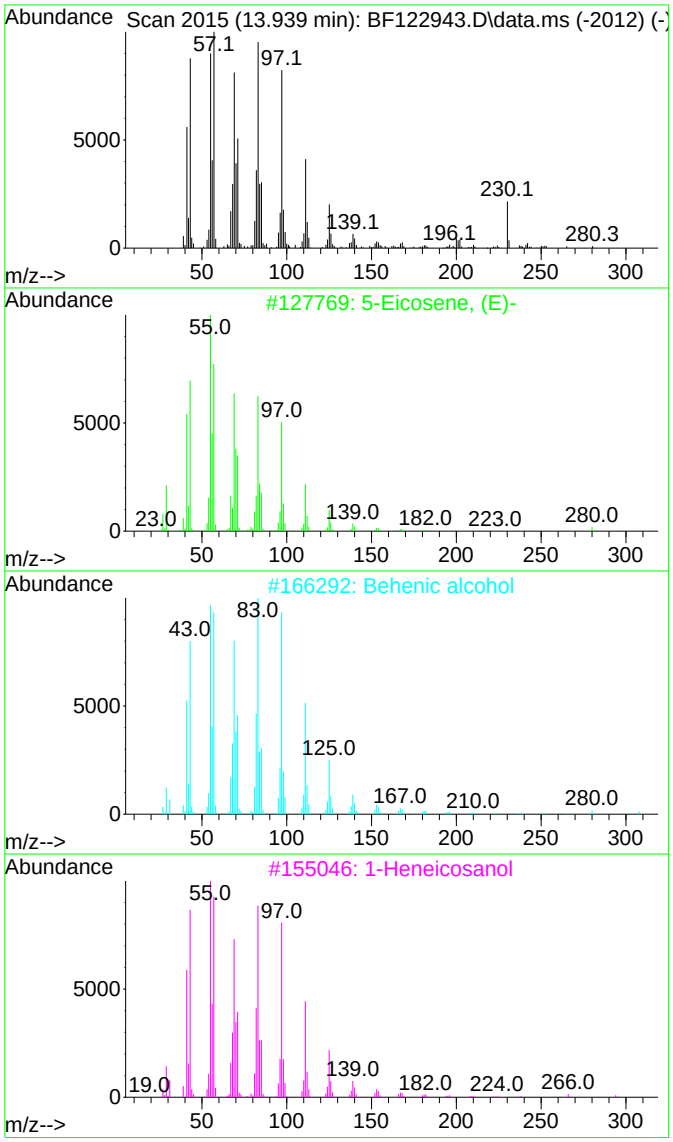
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

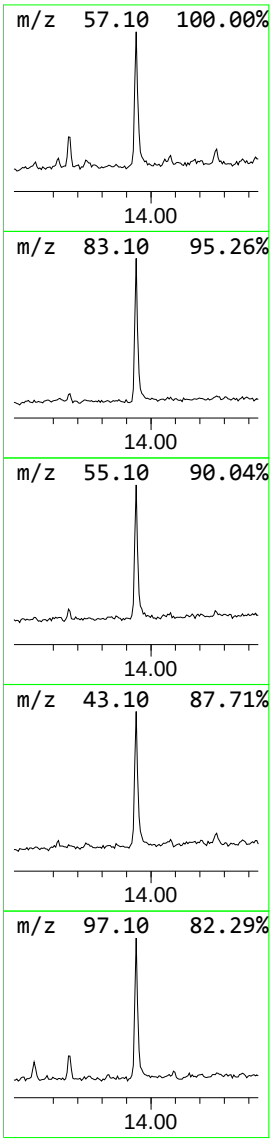
****

Peak Number 5 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	5.92 ng	478932	Chrysene-d12	14.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5	1-Heptacosanol	396	C27H56O	002004-39-9	91





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Sample : M1044-19
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

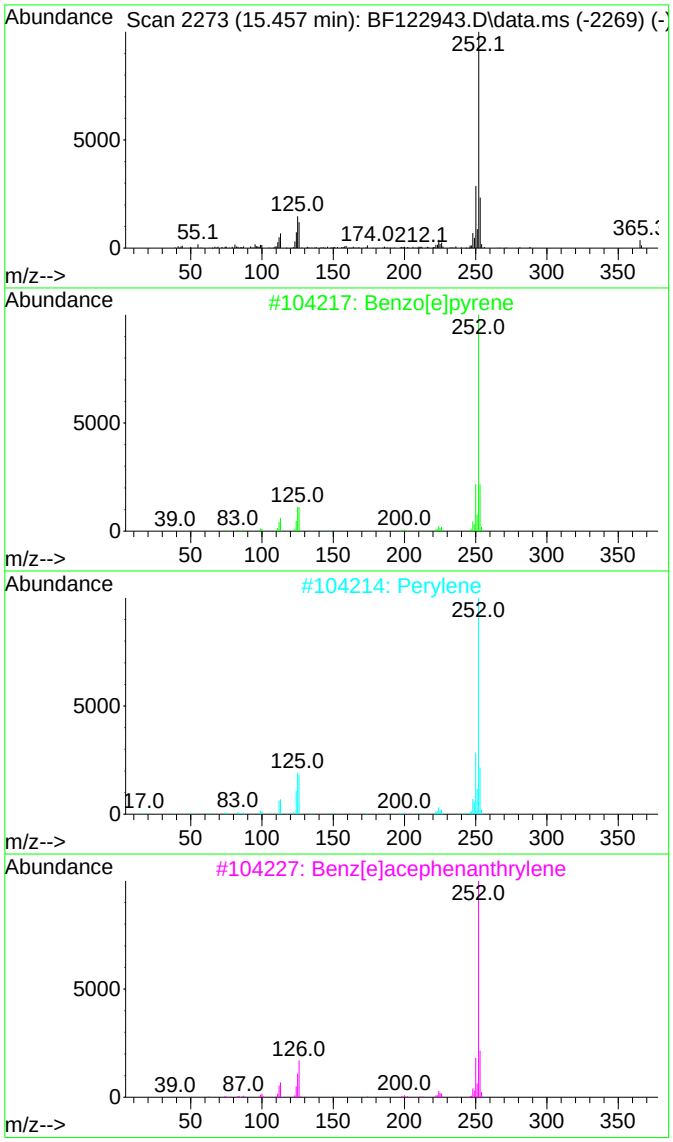
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

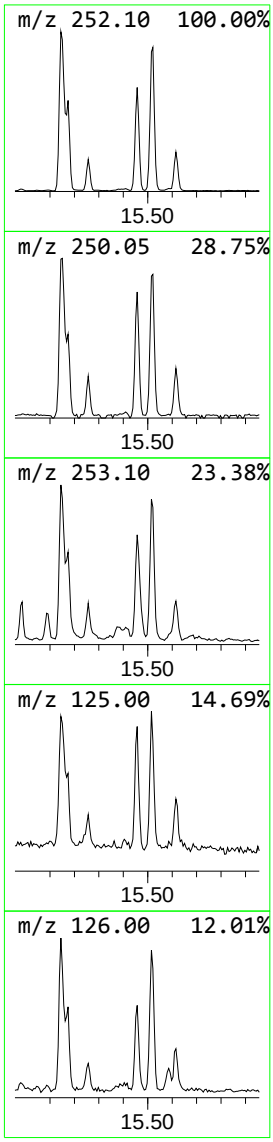
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.457	3.60 ng	214759	Perylene-d12	15.586

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Perylene	252	C20H12	000198-55-0	98
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93





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Acq On : 8 Jan 2021 16:28
Operator : JU/CG
Sample : M1044-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-12

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

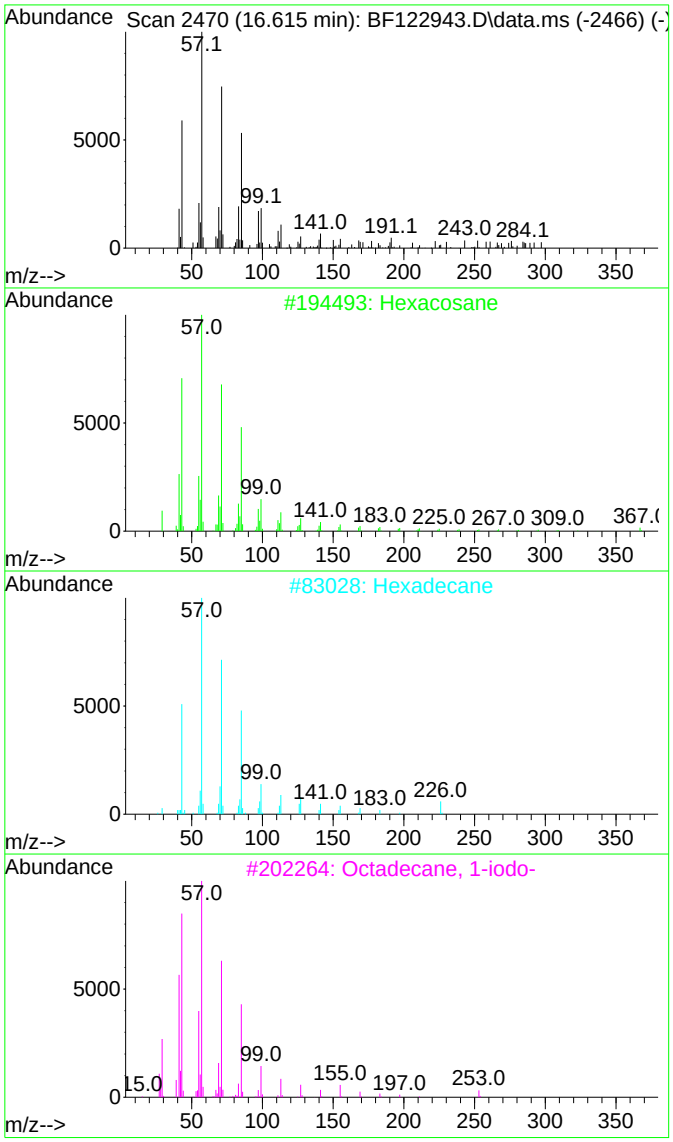
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

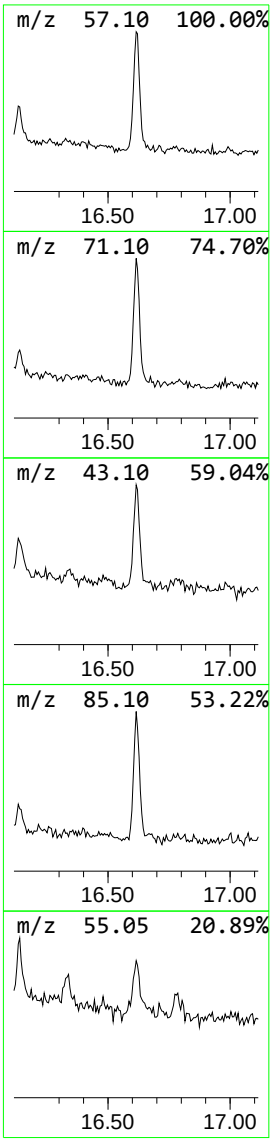
****

Peak Number 7 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.615	2.12 ng	126474	Perylene-d12	15.586

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	78
2	Hexadecane	226	C16H34	000544-76-3	72
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	72
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010821\
Data File : BF122943.D
Acq On : 8 Jan 2021 16:28
Operator : JU/CG
Sample : M1044-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-12

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...	2.222	12.1	ng	576252	1	6.916	954235	20.0
2-Pentanone, 4-...	5.134	6.8	ng	322464	1	6.916	954235	20.0
n-Hexadecanoic ...	11.974	3.0	ng	224837	4	11.445	1512000	20.0
2,4,4,6,6,8,8-H...	12.433	2.8	ng	213694	4	11.445	1512000	20.0
5-Eicosene, (E)-	13.939	5.9	ng	478932	5	14.098	1618740	20.0
Benzo[e]pyrene	15.457	3.6	ng	214759	6	15.586	1193270	20.0
Hexacosane	16.615	2.1	ng	126474	6	15.586	1193270	20.0