LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123091.D
Acq On : 29 Jan 2021 19:49
Operator : JU/CG
Sample : M1263-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0048-042-COMP-B-ELUTRIATE

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-BF012721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123091.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	12	18	24	rBV	1864386	2370322	31.25%	3.935%
2	5.504	577	581	584	rBV	3508678	3185585	42.00%	5.289%
3	6.504	747	751	762	rBV2	2411330	2643901	34.86%	4.390%
4	6.716	784	787	793	rBV	175615	185971	2.45%	0.309%
5	6.892	813	817	820	rBV	1809753	1494146	19.70%	2.481%
6	7.451	906	912	915	rBV	3678187	3944859	52.02%	6.550%
7	7.651	943	946	950	rVB	93468	88970	1.17%	0.148%
8	8.175	1030	1035	1038	rBV	2275509	1946444	25.67%	3.232%
9	9.257	1213	1219	1222	rBV	6715423	6990598	92.18%	11.607%
10	9.333	1229	1232	1234	rBV2	127136	122971	1.62%	0.204%
11	9.369	1234	1238	1255	rVB	1319329	1555709	20.51%	2.583%
12	9.645	1281	1285	1289	rBV	516920	429955	5.67%	0.714%
13	9.933	1327	1334	1338	rBV	2562634	2323249	30.63%	3.857%
14	10.527	1431	1435	1451	rBV	527089	1158385	15.27%	1.923%
15	10.727	1463	1469	1472	rBV	4696538	4656573	61.40%	7.731%
16	10.998	1512	1515	1517	rVB	108356	84623	1.12%	0.141%
17	11.427	1583	1588	1591	rBV	2424235	2365446	31.19%	3.927%
18	11.474	1593	1596	1600	rVB2	71221	81193	1.07%	0.135%
19	11.957	1671	1678	1681	rBV	1968809	2071365	27.31%	3.439%
20	11.986	1681	1683	1687	rVB	573500	496156	6.54%	0.824%
21	12.251	1725	1728	1732	rBV	141652	151224	1.99%	0.251%
22	12.410	1751	1755	1758	rBV	1107043	897049	11.83%	1.489%
23	12.468	1761	1765	1768	rVV	278752	271469	3.58%	0.451%
24	12.510	1768	1772	1788	rVB4	282398	812843	10.72%	1.350%
25	12.674	1796	1800	1804	rVB	466126	458357	6.04%	0.761%
26	12.745	1808	1812	1818	rBV	1034960	1034548	13.64%	1.718%
27	12.815	1821	1824	1827	rVV	269440	219107	2.89%	0.364%
28	13.021	1854	1859	1862	rBV	7622749	7583942	100.00%	12.592%
29	13.168	1880	1884	1888	rBV	131478	127527	1.68%	0.212%
30	13.251	1895	1898	1900	rBV	76891	75846	1.00%	0.126%
31	13.286	1900	1904	1907	rVV4	77272	141332	1.86%	0.235%
32	13.468	1932	1935	1937	rBV	79806	83248	1.10%	0.138%
33	13.498	1937	1940	1944	rVB	264641	270406	3.57%	0.449%
34	13.592	1954	1956	1959	rVV	97821	77608	1.02%	0.129%
35	13.639	1961	1964	1967	rVV	1071332	888273	11.71%	1.475%
36	13.674	1967	1970	1973	rVV2	264487	245125	3.23%	0.407%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123091.D
Acq On : 29 Jan 2021 19:49
Operator : JU/CG
Sample : M1263-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0048-042-COMP-B-ELUTRIATE

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-BF012721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.715	1974	1977	1983	rVB2	110860	125947	1.66%	0.209%
38	13.945	2010	2016	2029	rBV3	809806	2888976	38.09%	4.797%
39	14.074	2033	2038	2042	rVB	2333475	2076505	27.38%	3.448%
40	14.245	2063	2067	2070	rBV	150885	135326	1.78%	0.225%
41	14.551	2114	2119	2122	rBV	193975	175561	2.31%	0.291%
42	14.627	2124	2132	2142	rVV8	51942	201140	2.65%	0.334%
43	14.709	2143	2146	2155	rVB	157712	159830	2.11%	0.265%
44	14.862	2168	2172	2180	rVB	204624	207578	2.74%	0.345%
45	14.939	2182	2185	2190	rVB	119549	119416	1.57%	0.198%
46	15.209	2227	2231	2238	rVB	215095	232927	3.07%	0.387%
47	15.562	2285	2291	2295	rBV	1271647	1613365	21.27%	2.679%
48	15.603	2295	2298	2305	rVB	166048	219751	2.90%	0.365%
49	16.050	2369	2374	2382	rVB	129154	187539	2.47%	0.311%
50	16.174	2388	2395	2399	rBV4	86749	222545	2.93%	0.369%
51	16.574	2457	2463	2473	rVB3	66603	128903	1.70%	0.214%

Sum of corrected areas: 60229634

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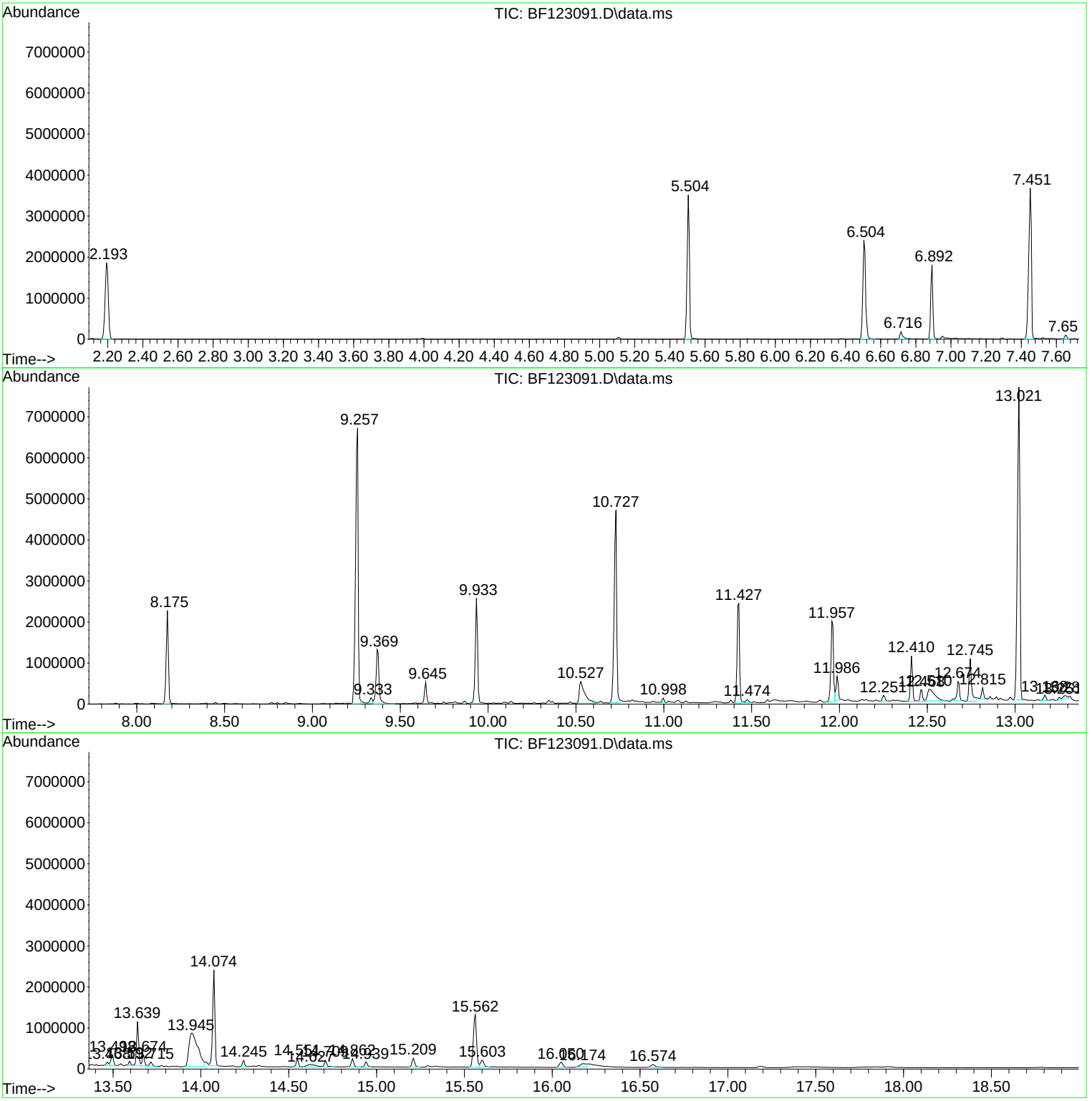
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0048-042-COMP-B-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.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\BF012921\
Data File : BF123091.D
Acq On : 29 Jan 2021 19:49
Operator : JU/CG
Sample : M1263-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0048-042-COMP-B-ELUTRIATE

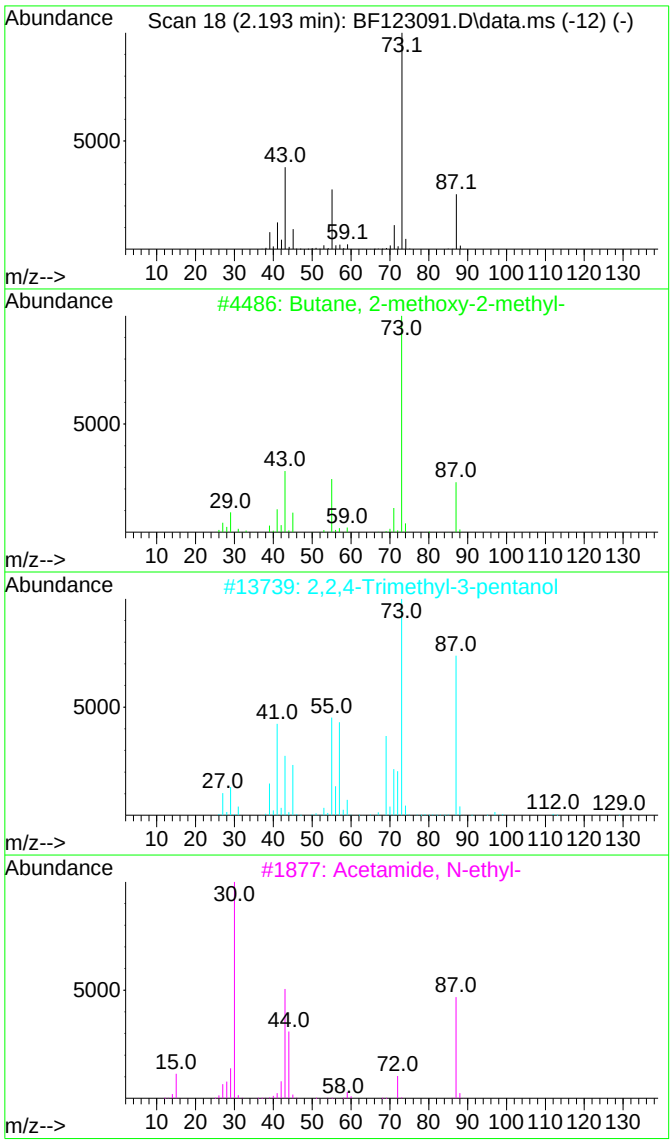
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

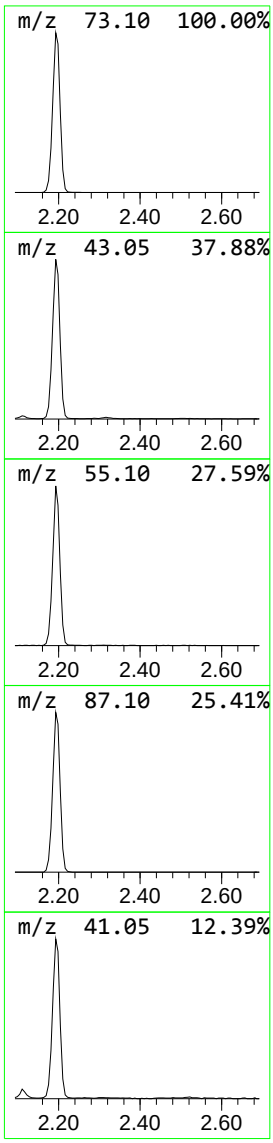
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	31.73 ng	2370320	1,4-Dichlorobenzene-d4	6.892

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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Operator : JU/CG
Sample : M1263-04
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0048-042-COMP-B-ELUTRIATE

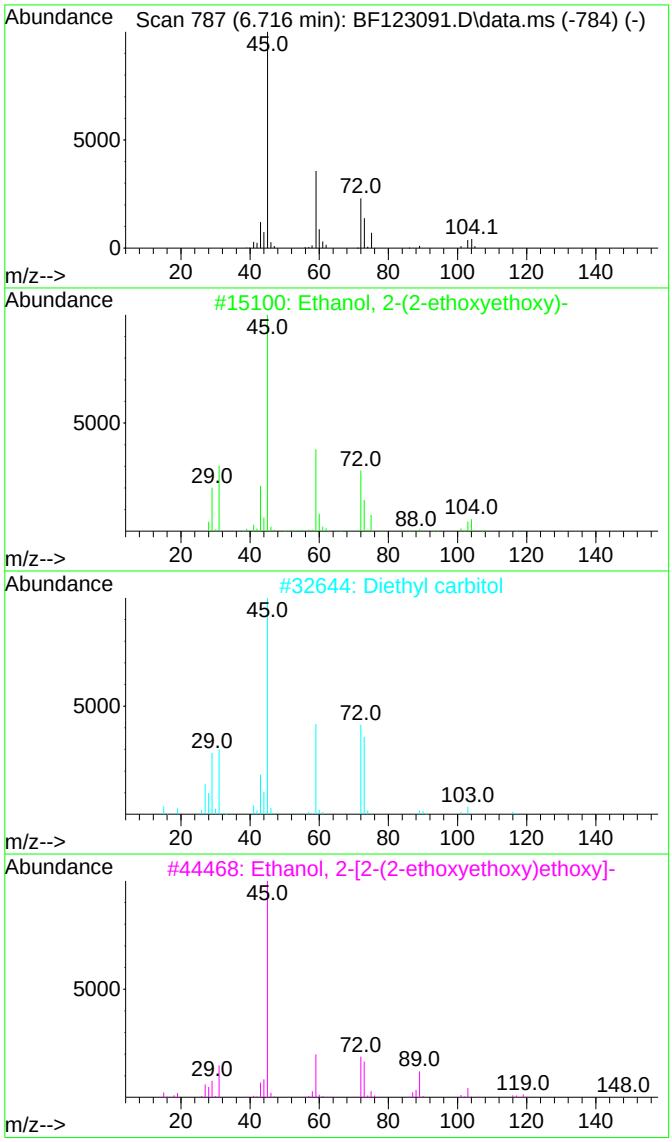
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

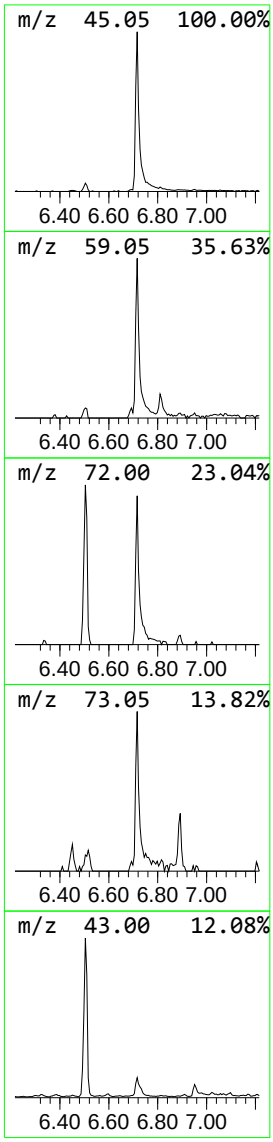
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.716	2.49 ng	185971	1,4-Dichlorobenzene-d4	6.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2	Diethyl carbitol	162	C8H18O3	000112-36-7	72
3	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	64
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	50
5	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123091.D
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Operator : JU/CG
Sample : M1263-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0048-042-COMP-B-ELUTRIATE

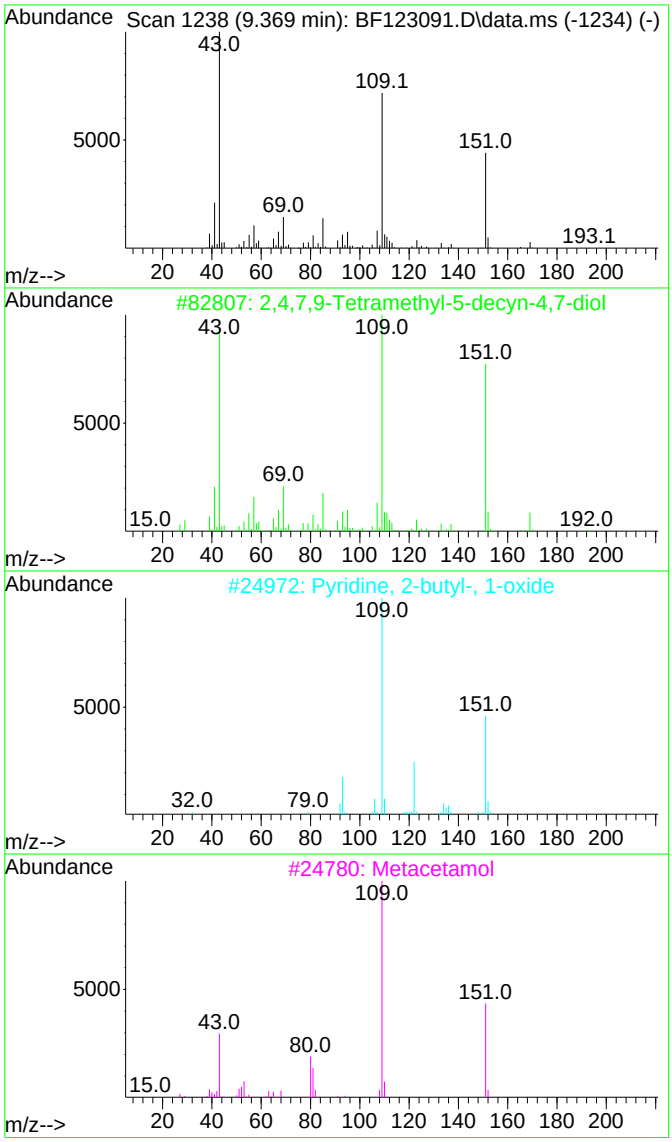
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

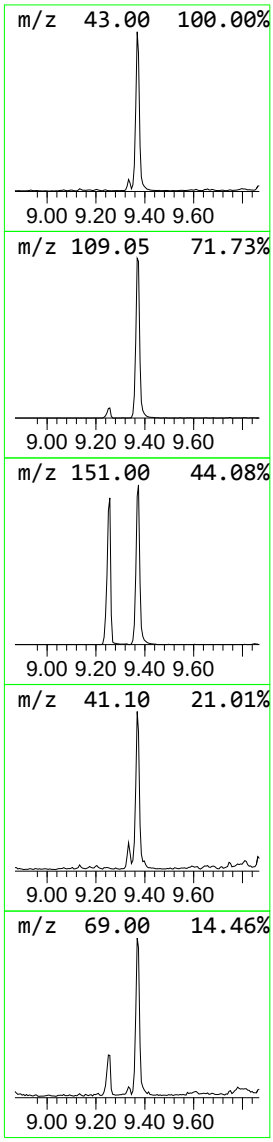
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.369	13.39 ng	1555710	Acenaphthene-d10	9.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
3	Metacetamol	151	C8H9NO2	000621-42-1	53
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53
5	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123091.D
Acq On : 29 Jan 2021 19:49
Operator : JU/CG
Sample : M1263-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0048-042-COMP-B-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

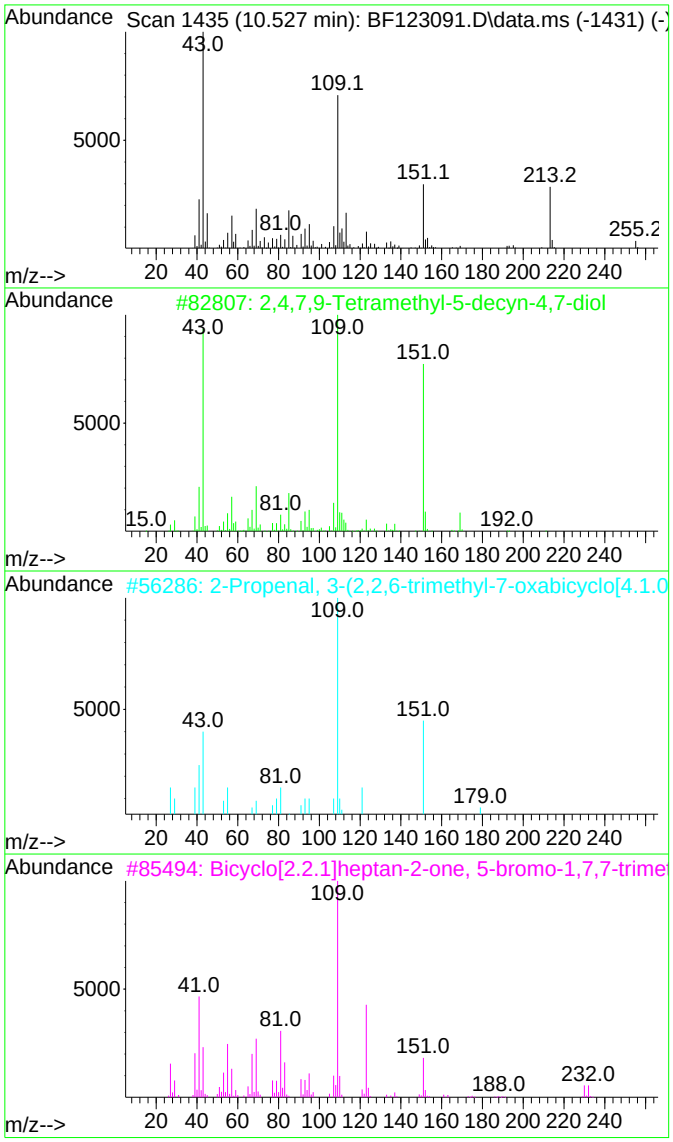
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

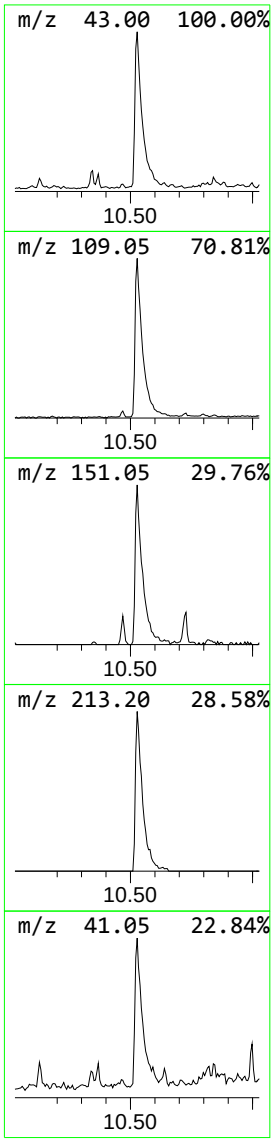
****

Peak Number 4 unknown10.527 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.527	9.97 ng	1158390	Acenaphthene-d10	9.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	58
2	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	38
3	Bicyclo[2.2.1]heptan-2-one, 5-br...	230	C10H15BrO	010293-00-2	32
4	Acetaminophen	151	C8H9NO2	000103-90-2	30
5	Metacetamol	151	C8H9NO2	000621-42-1	30





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Acq On : 29 Jan 2021 19:49
Operator : JU/CG
Sample : M1263-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0048-042-COMP-B-ELUTRIATE

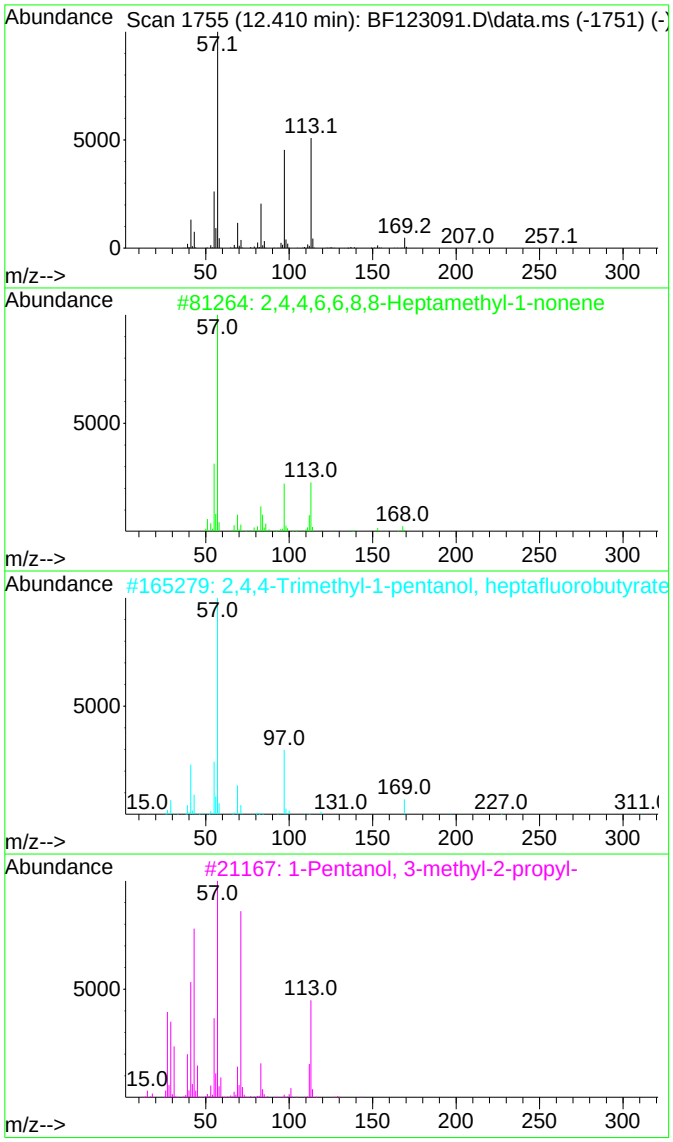
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

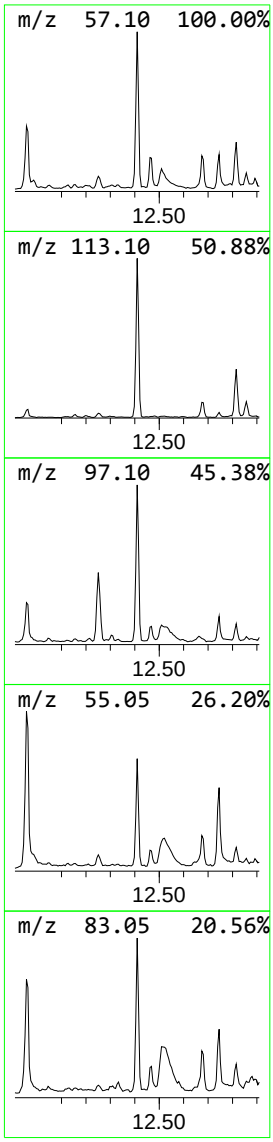
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	7.58 ng	897049	Phenanthrene-d10	11.427

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, hept...	326	C12H17F7O2	1000365-01-4	43
3	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	40
4	Vardenafil	488	C23H32N6O4S	224785-90-4	16
5	3-Methylpentyl ethylphosphonoflu...	196	C8H18FO2P	1000298-39-1	16





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Instrument :
BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

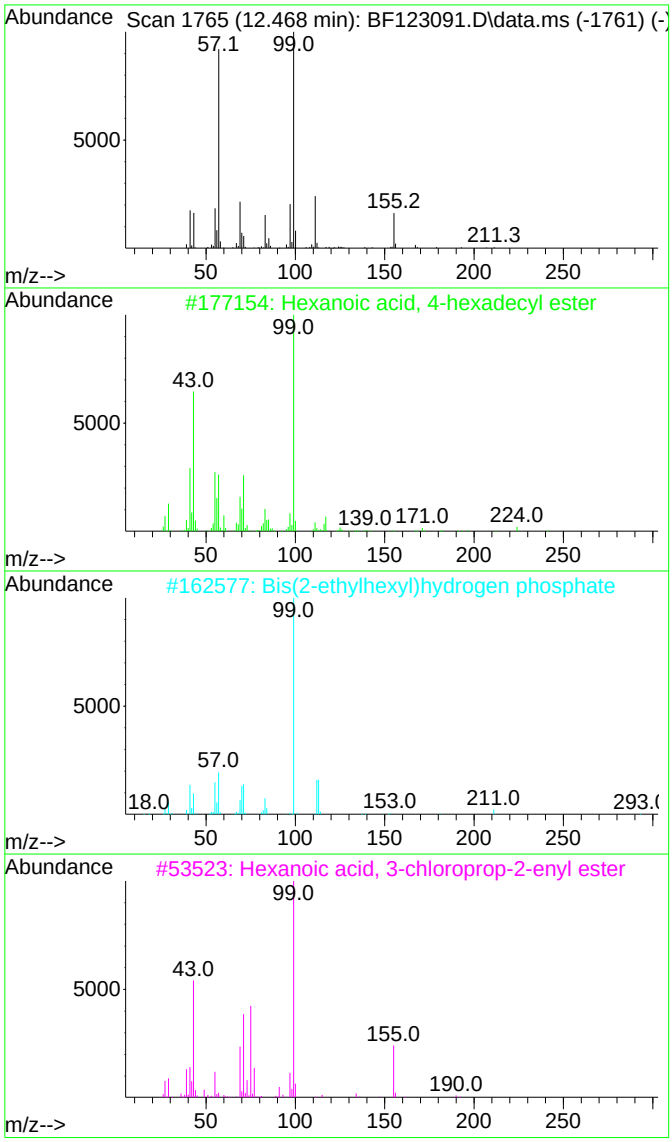
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

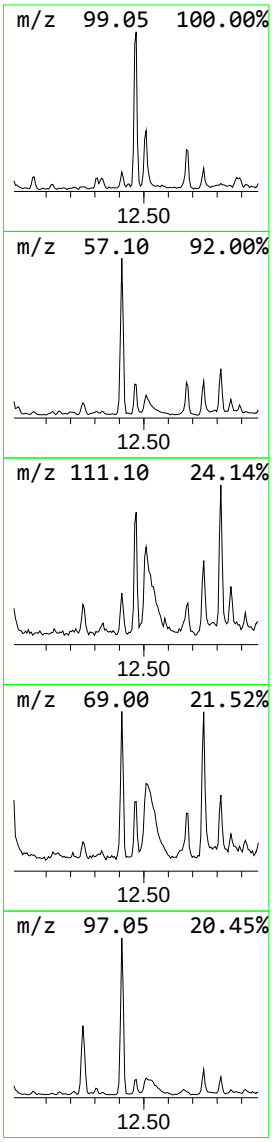
****

Peak Number 6 unknown12.468 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.468	2.30 ng	271469	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 4-hexadecyl ester	340	C22H44O2	1000282-83-8	38
2	Bis(2-ethylhexyl)hydrogen phosphate	322	C16H35O4P	000298-07-7	37
3	Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	37
4	Hexanoic acid, 5-tridecyl ester	298	C19H38O2	1000279-29-4	36
5	2-Propylthiazole	127	C6H9NS	017626-75-4	35





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Instrument :
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0048-042-COMP-B-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

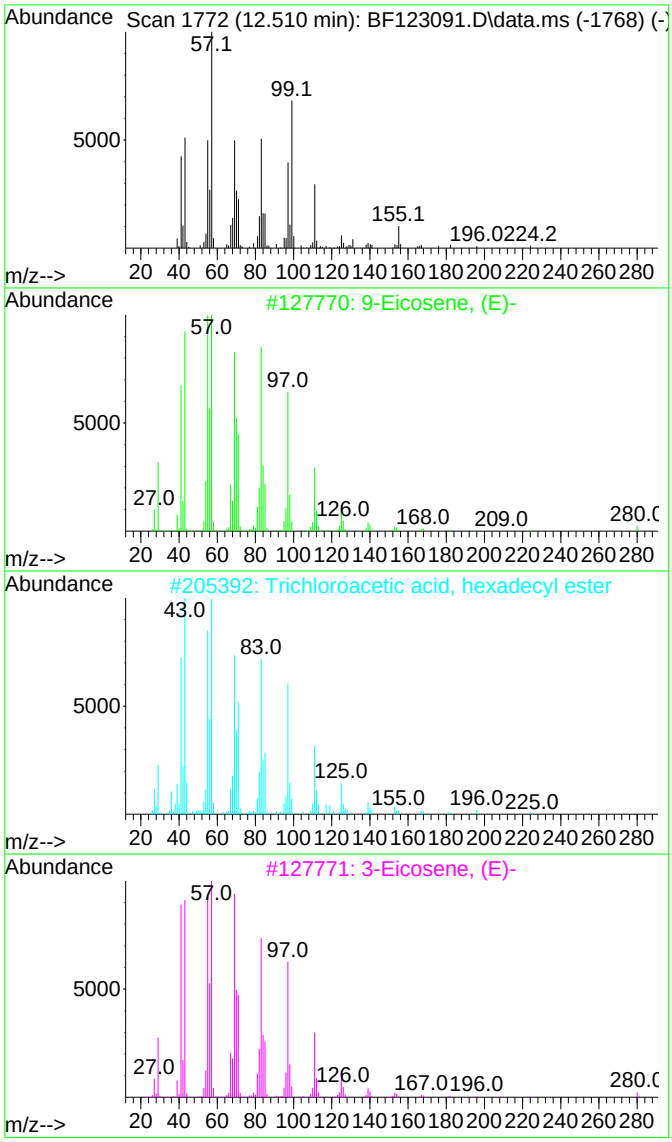
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

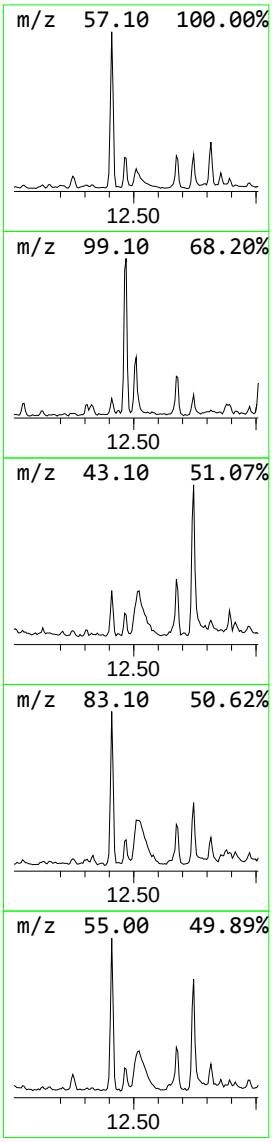
****

Peak Number 7 9-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.509	6.87 ng	812843	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Eicosene, (E)-	280	C20H40	074685-29-3	62
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	47
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	46
4	Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	46
5	Cetene	224	C16H32	000629-73-2	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123091.D
Acq On : 29 Jan 2021 19:49
Operator : JU/CG
Sample : M1263-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0048-042-COMP-B-ELUTRIATE

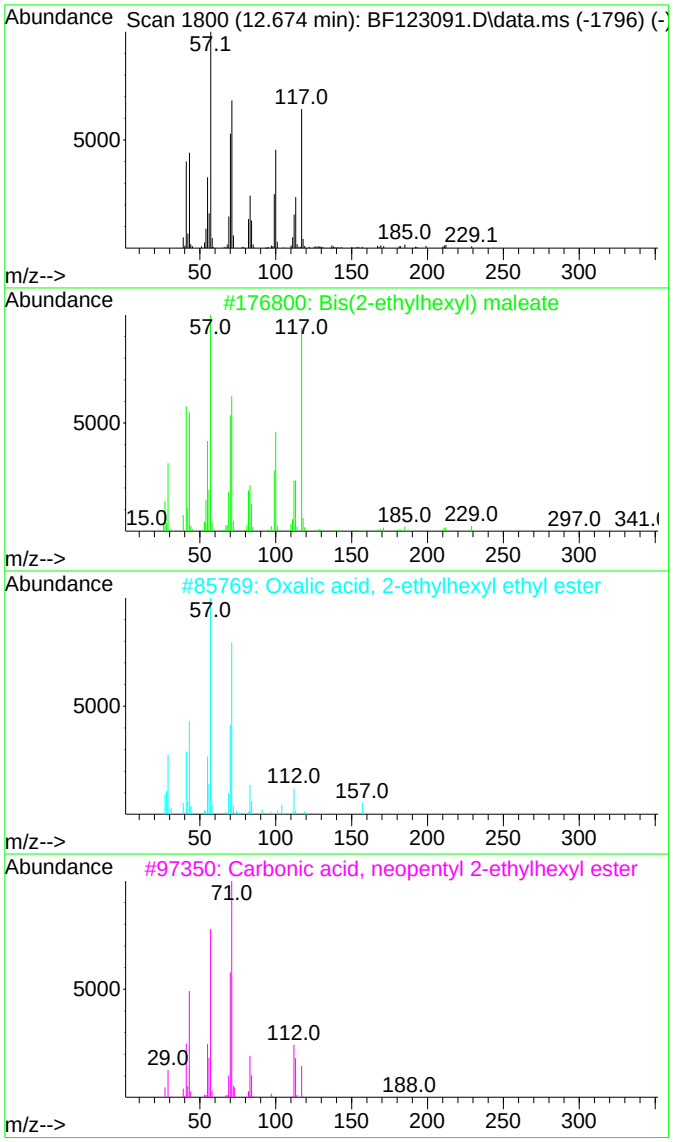
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

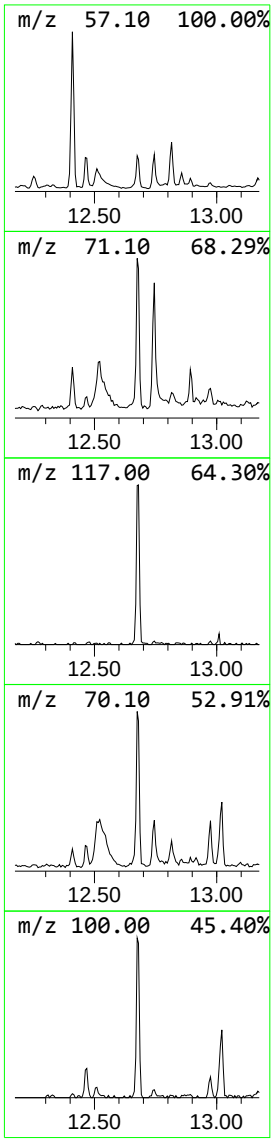
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Bis(2-ethylhexyl) maleate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.674	3.88 ng	458357	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bis(2-ethylhexyl) maleate	340	C20H36O4	000142-16-5	62
2	Oxalic acid, 2-ethylhexyl ethyl ...	230	C12H22O4	1000309-38-4	38
3	Carbonic acid, neopentyl 2-ethyl...	244	C14H28O3	1000357-85-7	38
4	2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	35
5	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	35





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Data File : BF123091.D
Acq On : 29 Jan 2021 19:49
Operator : JU/CG
Sample : M1263-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0048-042-COMP-B-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

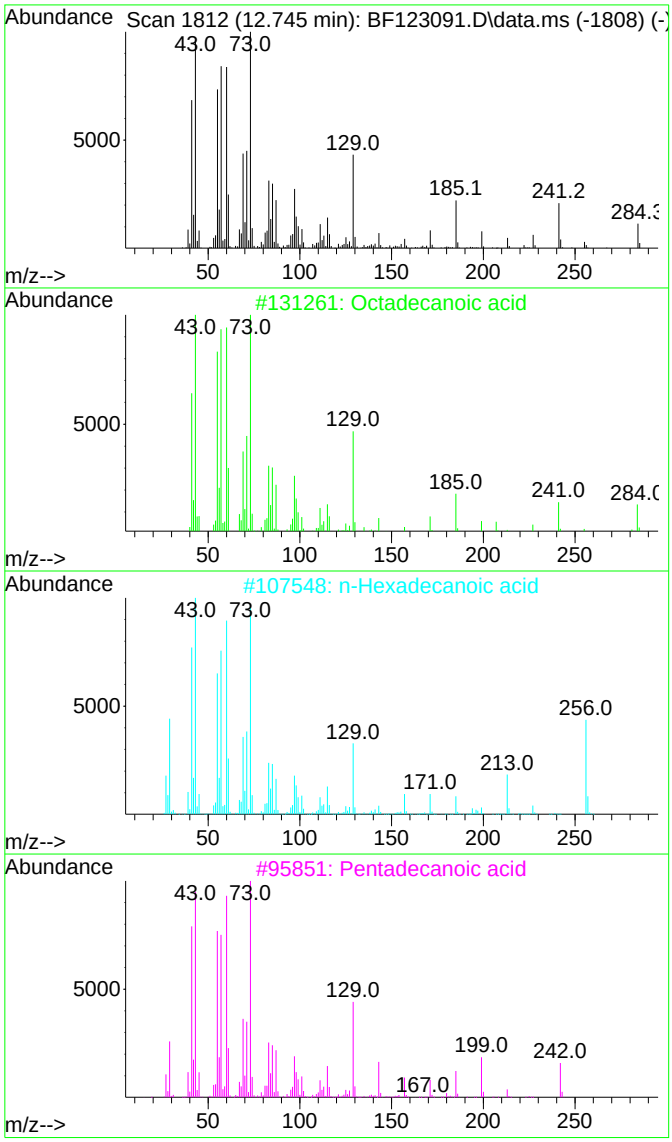
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

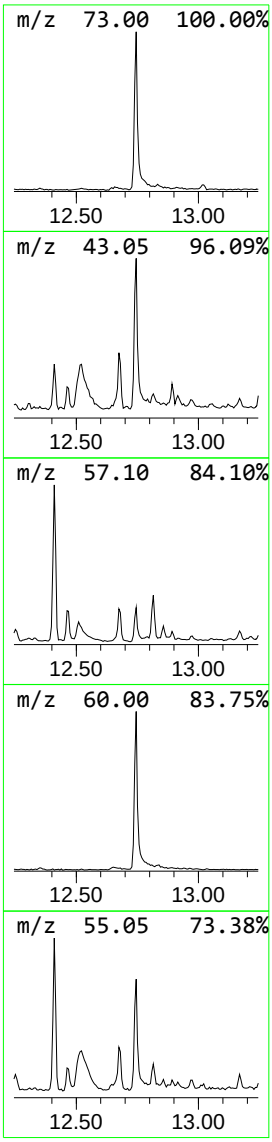
****

Peak Number 9 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.745	8.75 ng	1034550	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Tridecanoic acid	214	C13H26O2	000638-53-9	74





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Sample : M1263-04
Misc :
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Instrument :
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ClientSampleId :
0048-042-COMP-B-ELUTRIATE

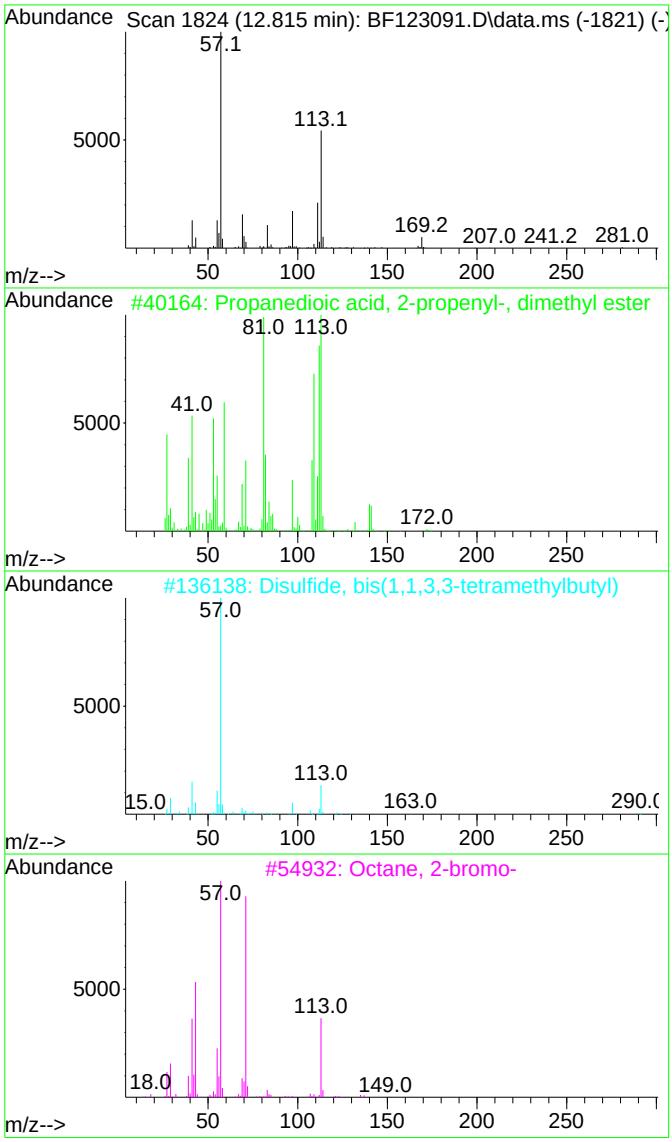
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

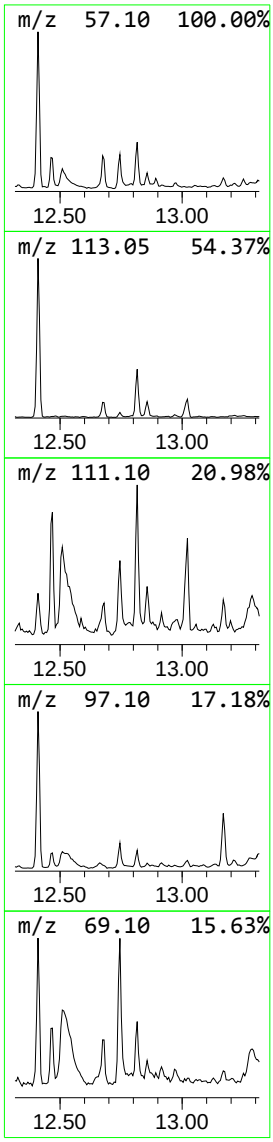
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 unknown12.815 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.815	2.11 ng	219107	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanedioic acid, 2-propenyl-, ...	172	C8H12O4	040637-56-7	47
2	Disulfide, bis(1,1,3,3-tetrameth...	290	C16H34S2	029956-99-8	38
3	Octane, 2-bromo-	192	C8H17Br	000557-35-7	37
4	3-(4-Methyl-2,5-dioxo-4-imidazol...	186	C7H10N2O4	007511-46-8	27
5	1-Isopropylbutyl ethylphosphonof...	210	C9H20FO2P	1000298-39-8	27





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Sample : M1263-04
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
0048-042-COMP-B-ELUTRIATE

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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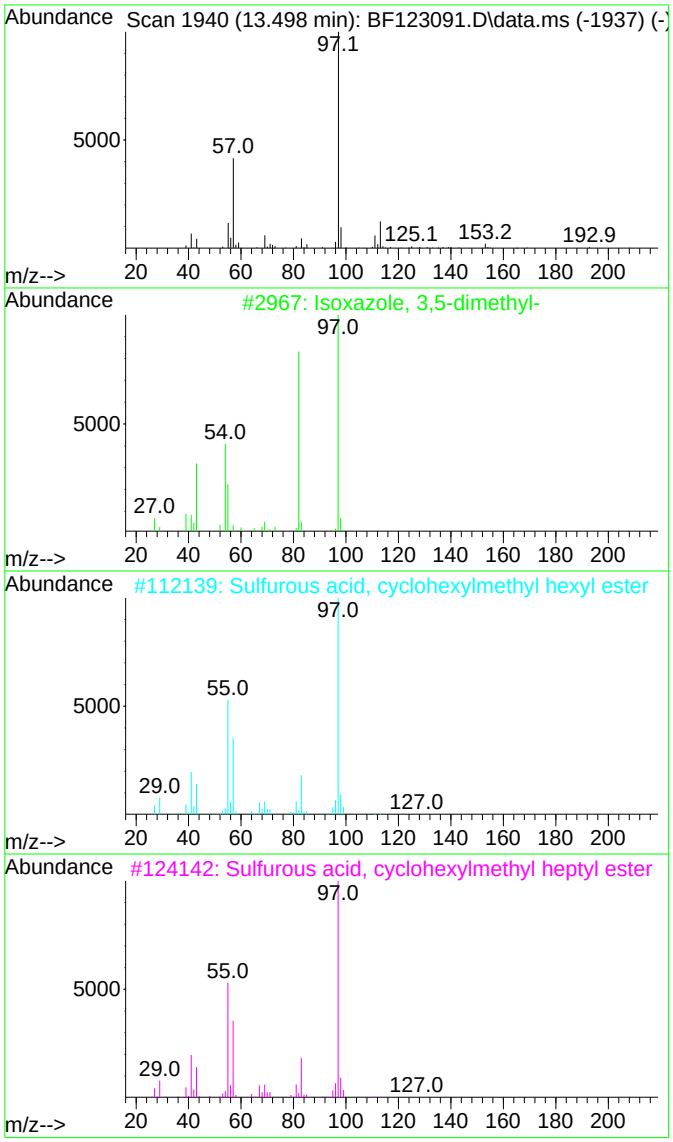
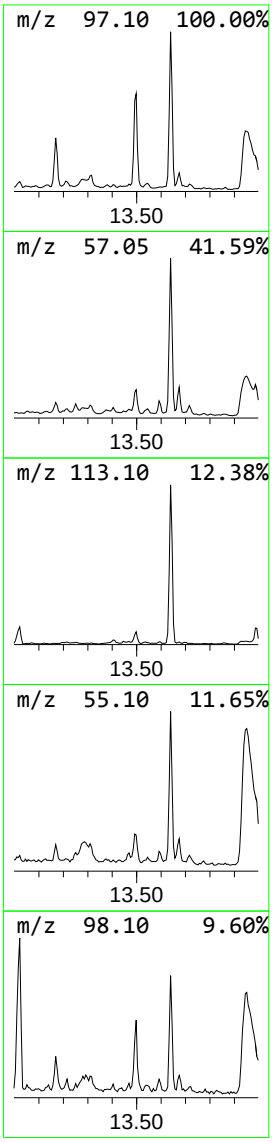
Peak Number 11 Isoxazole, 3,5-dimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.498	2.60 ng	270406	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	59
2	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-6	39
3	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	38
4	1-(Trimethylsilyl)-1-propyne	112	C6H12Si	006224-91-5	38
5	1,1-Dimethyl-1-silacyclo-3-pentene	112	C6H12Si	016054-12-9	36





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Sample : M1263-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
0048-042-COMP-B-ELUTRIATE

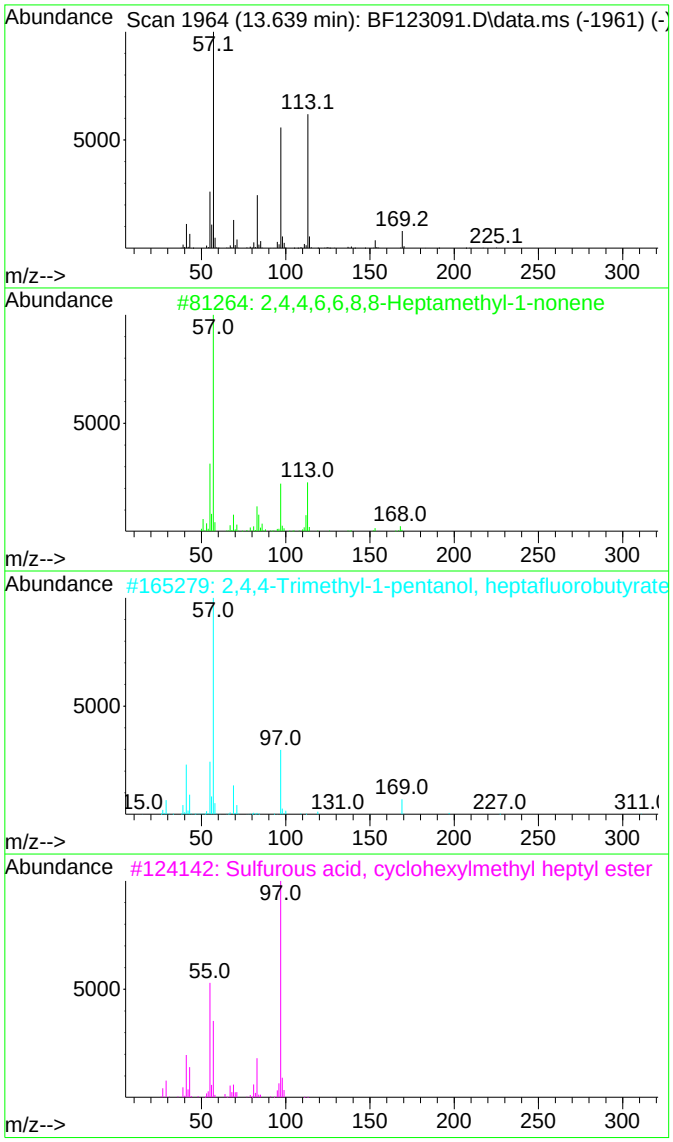
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

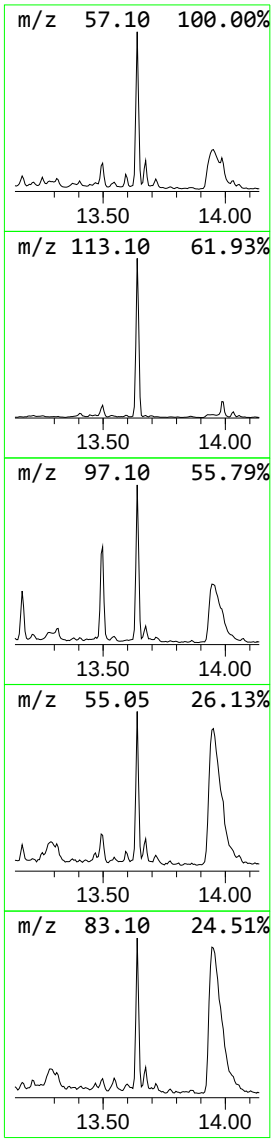
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 unknown13.639 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.639	8.56 ng	888273	Chrysene-d12	14.074

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	64
2	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	37
3	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	37
4	5-Nonanone, 2,2,8,8-tetramethyl-	198	C13H26O	005709-95-5	32
5	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	27





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Sample : M1263-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
0048-042-COMP-B-ELUTRIATE

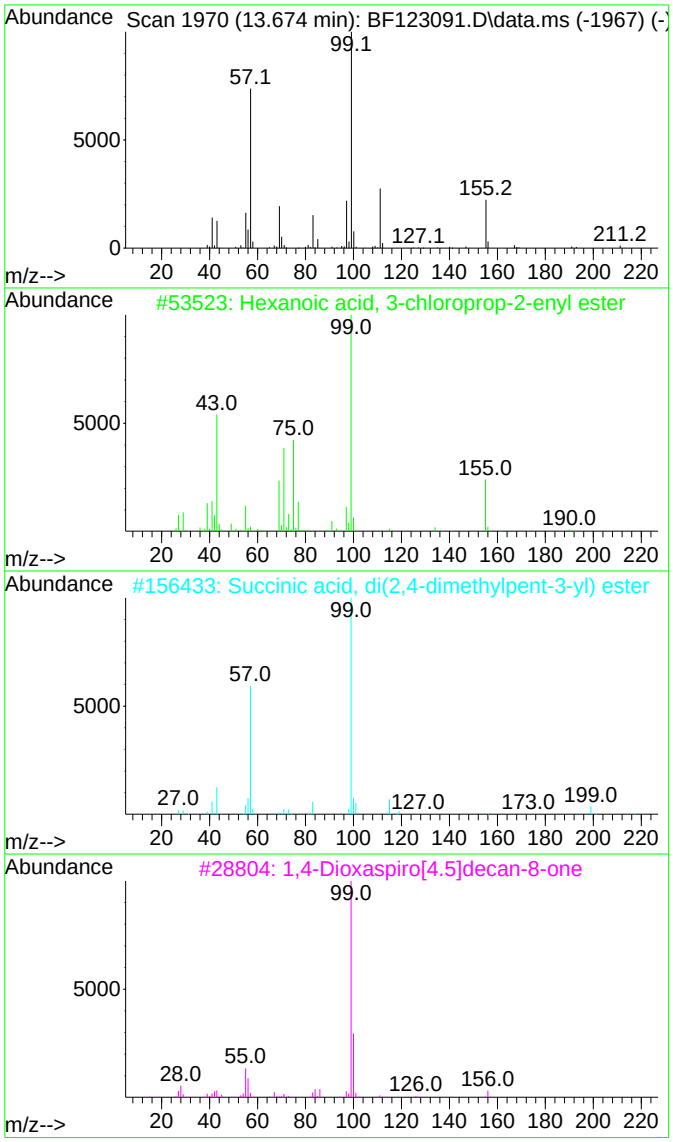
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

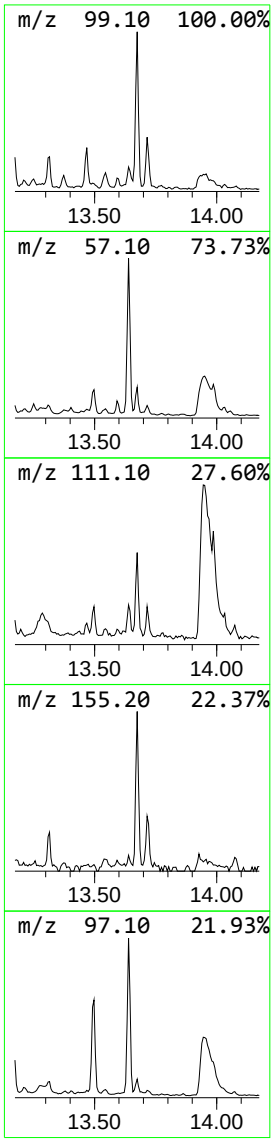
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 unknown13.674 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.674	2.36 ng	245125	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	38
2	Succinic acid, di(2,4-dimethylpe...	314	C18H34O4	1000349-36-7	38
3	1,4-Dioxaspiro[4.5]decan-8-one	156	C8H12O3	004746-97-8	35
4	Hexanoic acid, 5-tridecyl ester	298	C19H38O2	1000279-29-4	33
5	4-Methyl-3,5-decandione	184	C11H20O2	1000374-13-1	28





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Sample : M1263-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
0048-042-COMP-B-ELUTRIATE

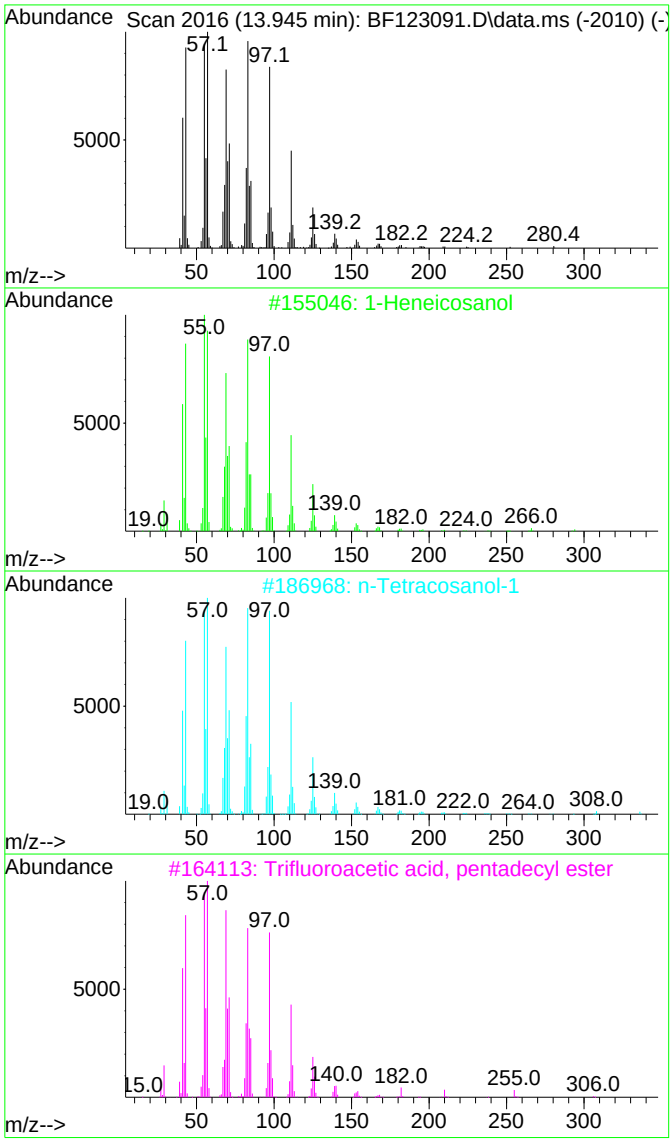
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

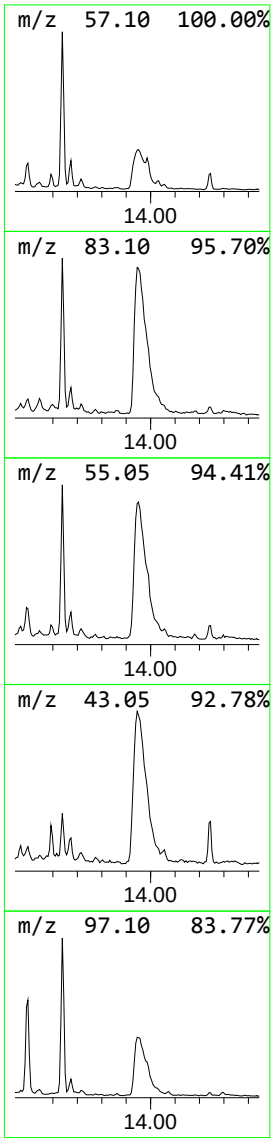
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	27.83 ng	2888980	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94





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Operator : JU/CG
Sample : M1263-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
0048-042-COMP-B-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.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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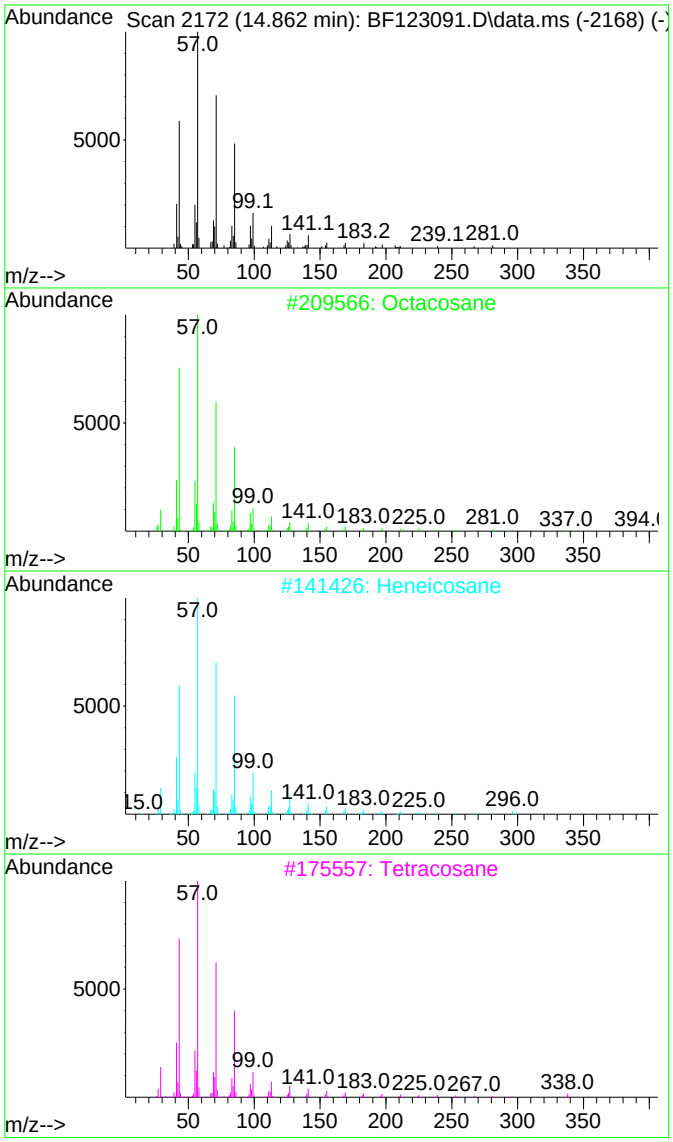
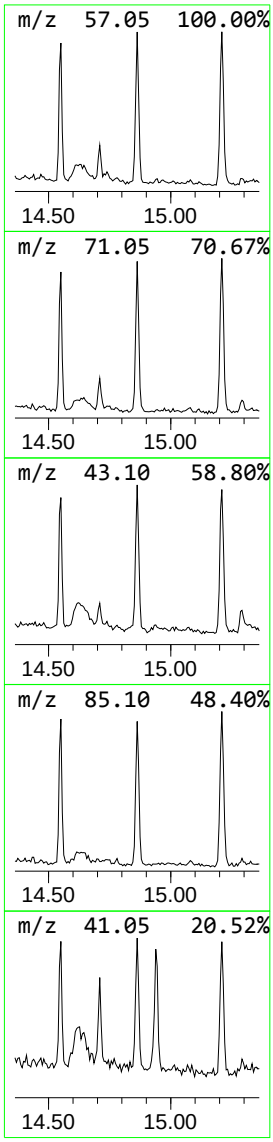
Peak Number 15 Octacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.862	2.57 ng	207578	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Pentacosane	352	C25H52	000629-99-2	87
5	Eicosane	282	C20H42	000112-95-8	86





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Data File : BF123091.D
Acq On : 29 Jan 2021 19:49
Operator : JU/CG
Sample : M1263-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0048-042-COMP-B-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.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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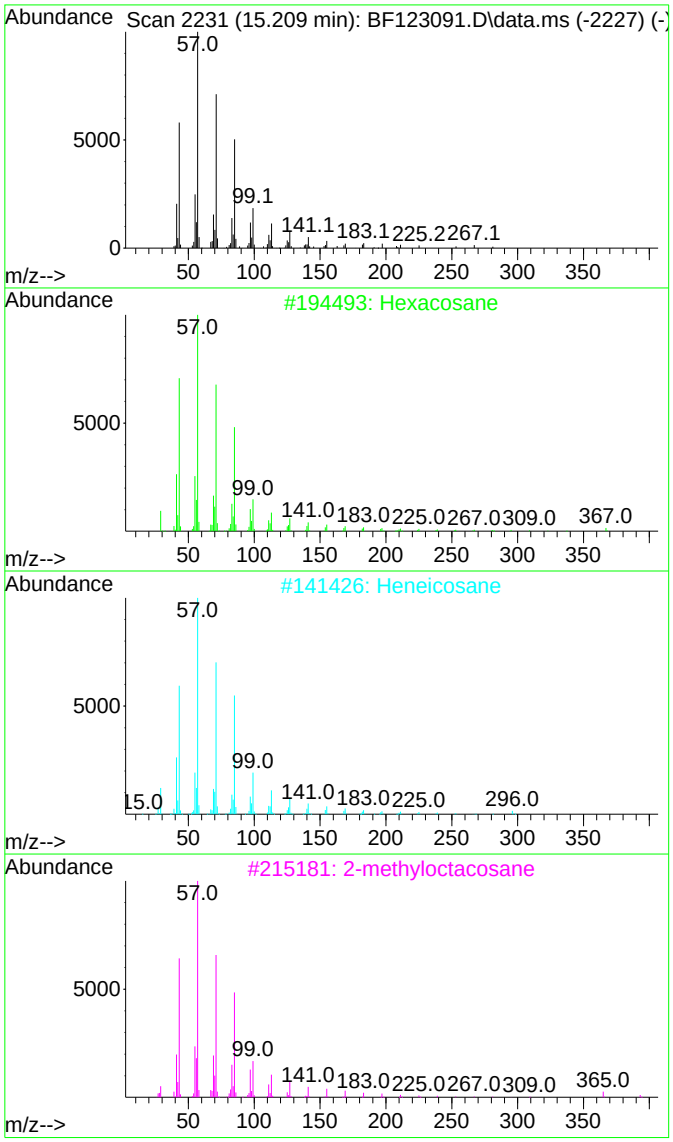
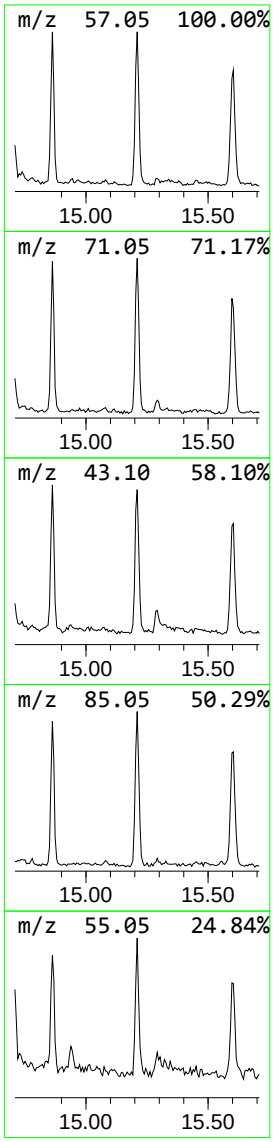
Peak Number 16 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.209	2.89 ng	232927	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Hentriacontane	437	C31H64	000630-04-6	91
5	Octacosane	394	C28H58	000630-02-4	90





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Sample : M1263-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
0048-042-COMP-B-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.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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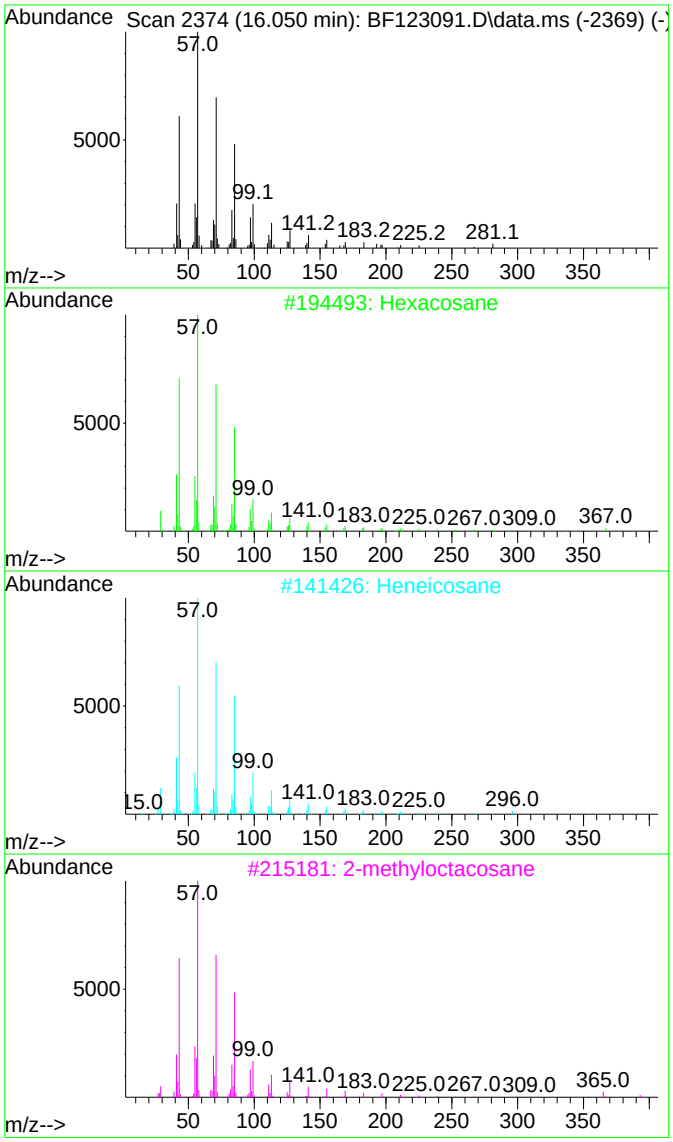
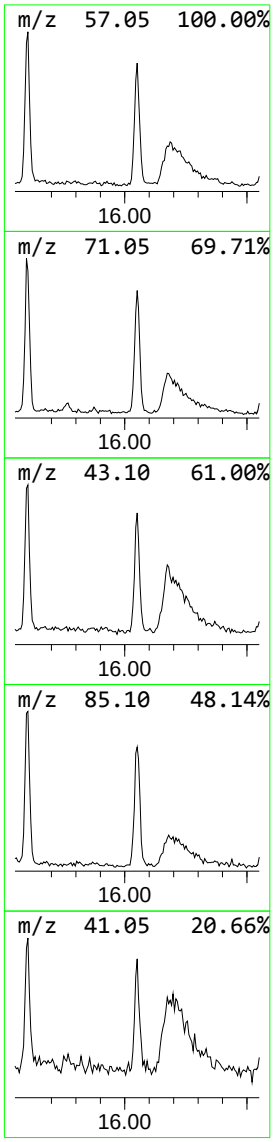
Peak Number 17 Heneicosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.051	2.32 ng	187539	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	2-methyltetracosane	352	C25H52	1000376-72-6	90
5	Octacosane	394	C28H58	000630-02-4	87





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Sample : M1263-04
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ALS Vial : 20 Sample Multiplier: 1

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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.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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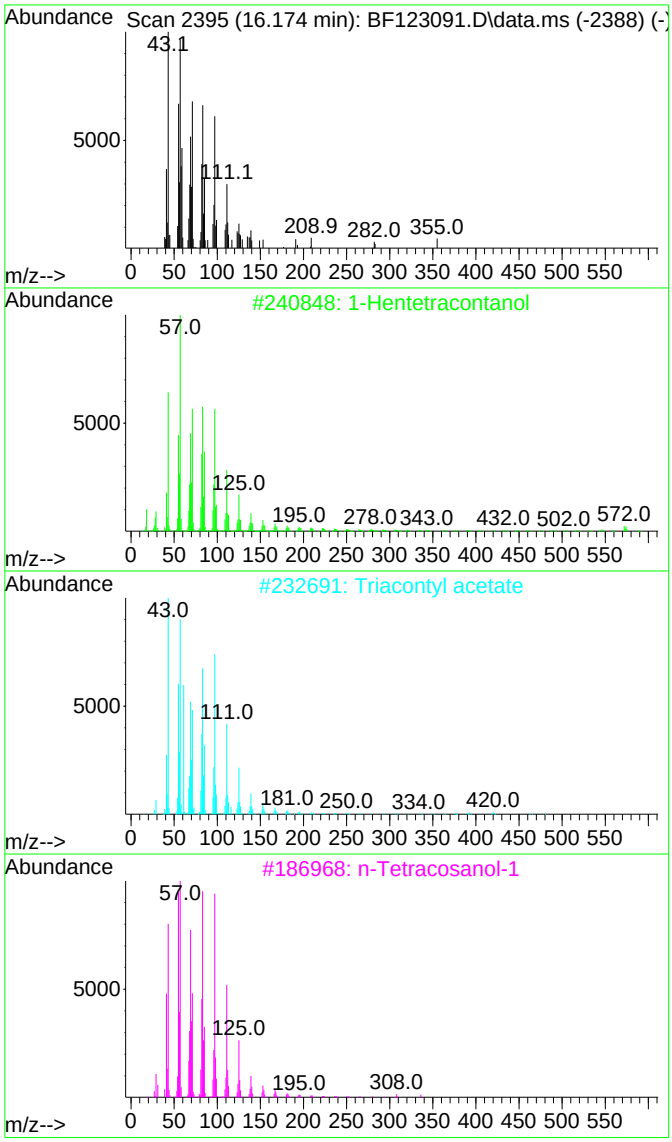
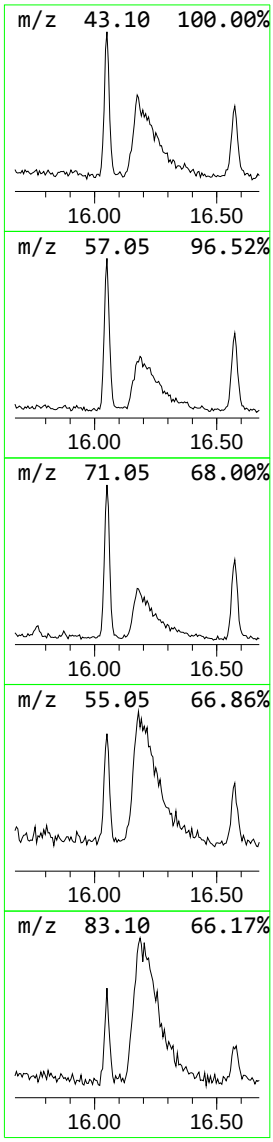
Peak Number 18 1-Hentetracontanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.174	2.76 ng	222545	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hentetracontanol	593	C41H84O	040710-42-7	70
2	Triacontyl acetate	480	C32H64O2	041755-58-2	70
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	60
4	Heptacosyl acetate	438	C29H58O2	1000351-78-2	58
5	17-Pentatriacontene	491	C35H70	006971-40-0	58





Tentatively Identified Compound (LSC) summary

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Data File : BF123091.D
Acq On : 29 Jan 2021 19:49
Operator : JU/CG
Sample : M1263-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0048-042-COMP-B-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.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...	2.193	31.7	ng	2370320	1	6.892	1494150	20.0
Ethanol, 2-(2-e...	6.716	2.5	ng	185971	1	6.892	1494150	20.0
2,4,7,9-Tetrame...	9.369	13.4	ng	1555710	3	9.933	2323250	20.0
unknown10.527	10.527	10.0	ng	1158390	3	9.933	2323250	20.0
2,4,4,6,6,8,8-H...	12.410	7.6	ng	897049	4	11.427	2365450	20.0
unknown12.468	12.468	2.3	ng	271469	4	11.427	2365450	20.0
9-Eicosene, (E)-	12.509	6.9	ng	812843	4	11.427	2365450	20.0
Bis(2-ethylhexy...	12.674	3.9	ng	458357	4	11.427	2365450	20.0
Octadecanoic acid	12.745	8.8	ng	1034550	4	11.427	2365450	20.0
unknown12.815	12.815	2.1	ng	219107	5	14.074	2076510	20.0
Isoxazole, 3,5-...	13.498	2.6	ng	270406	5	14.074	2076510	20.0
unknown13.639	13.639	8.6	ng	888273	5	14.074	2076510	20.0
unknown13.674	13.674	2.4	ng	245125	5	14.074	2076510	20.0
1-Heneicosanol	13.945	27.8	ng	2888980	5	14.074	2076510	20.0
Octacosane	14.862	2.6	ng	207578	6	15.562	1613370	20.0
Hexacosane	15.209	2.9	ng	232927	6	15.562	1613370	20.0
Heneicosane	16.051	2.3	ng	187539	6	15.562	1613370	20.0
1-Hentetracontanol	16.174	2.8	ng	222545	6	15.562	1613370	20.0