LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090721\
Data File : BF125386.D
Acq On : 7 Sep 2021 14:15
Operator : JU/CG
Sample : M3660-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ETGI-332

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125386.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.151	7	11	28	rVB	210614	390752	22.28%	2.017%
2	5.516	579	583	591	rBV	421971	442447	25.23%	2.283%
3	6.522	751	754	766	rBV	341599	392412	22.37%	2.025%
4	6.898	814	818	824	rBV	812985	693165	39.52%	3.577%
5	7.457	910	913	922	rVB	251698	236639	13.49%	1.221%
6	8.180	1032	1036	1042	rVB	867056	743679	42.40%	3.838%
7	9.251	1215	1218	1226	rBV	479509	411884	23.49%	2.126%
8	9.651	1282	1286	1293	rVB7	16370	31835	1.82%	0.164%
9	9.798	1305	1311	1315	rVV	61216	60271	3.44%	0.311%
10	9.933	1331	1334	1338	rBV	949433	766726	43.72%	3.957%
11	9.969	1338	1340	1342	rVB	36623	28630	1.63%	0.148%
12	10.139	1364	1369	1372	rVB3	29880	45159	2.57%	0.233%
13	10.480	1424	1427	1431	rVB	45648	44645	2.55%	0.230%
14	10.721	1465	1468	1478	rVB	290821	270207	15.41%	1.394%
15	10.839	1484	1488	1495	rVB6	30433	61679	3.52%	0.318%
16	10.921	1496	1502	1505	rBV5	14790	23514	1.34%	0.121%
17	11.027	1515	1520	1523	rBV4	22478	34388	1.96%	0.177%
18	11.063	1523	1526	1528	rBV4	16251	19437	1.11%	0.100%
19	11.274	1559	1562	1564	rBV3	30381	32518	1.85%	0.168%
20	11.316	1565	1569	1575	rVB3	25637	41411	2.36%	0.214%
21	11.421	1583	1587	1589	rBV	985875	825622	47.08%	4.261%
22	11.445	1589	1591	1595	rVV	408990	324869	18.52%	1.677%
23	11.498	1597	1600	1603	rVV	145698	113690	6.48%	0.587%
24	11.527	1603	1605	1609	rVV3	15931	23901	1.36%	0.123%
25	11.657	1623	1627	1632	rBV3	32670	46041	2.63%	0.238%
26	11.716	1633	1637	1641	rVV3	23392	37755	2.15%	0.195%
27	11.751	1641	1643	1648	rVB4	20800	27240	1.55%	0.141%
28	11.804	1649	1652	1655	rVB	32090	26780	1.53%	0.138%
29	11.939	1669	1675	1683	rBV4	298980	507670	28.95%	2.620%
30	11.998	1683	1685	1688	rVB	47634	39276	2.24%	0.203%
31	12.039	1688	1692	1694	rBV	132211	144323	8.23%	0.745%
32	12.110	1699	1704	1706	rBV4	38028	54477	3.11%	0.281%
33	12.157	1709	1712	1714	rBV4	22165	24048	1.37%	0.124%
34	12.215	1720	1722	1725	rBV	44810	41247	2.35%	0.213%
35	12.245	1725	1727	1730	rVB3	26882	20876	1.19%	0.108%
36	12.398	1750	1753	1755	rBV2	34562	33816	1.93%	0.175%

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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ETGI-332

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.421	1755	1757	1760	rVV	30739	36231	2.07%	0.187%
38	12.468	1762	1765	1767	rVV	105171	126634	7.22%	0.654%
39	12.492	1767	1769	1771	rVV2	120739	147632	8.42%	0.762%
40	12.510	1771	1772	1778	rVV3	144710	145605	8.30%	0.751%
41	12.557	1778	1780	1785	rVV2	56137	77146	4.40%	0.398%
42	12.633	1790	1793	1797	rVV	984116	907331	51.74%	4.682%
43	12.674	1797	1800	1802	rVV2	79003	78762	4.49%	0.406%
44	12.698	1802	1804	1806	rVV2	31724	29712	1.69%	0.153%
45	12.721	1806	1808	1812	rVB2	106017	122312	6.97%	0.631%
46	12.786	1817	1819	1821	rVB	32822	26482	1.51%	0.137%
47	12.810	1821	1823	1826	rVB4	26785	23571	1.34%	0.122%
48	12.868	1826	1833	1838	rBV	953281	1064960	60.72%	5.496%
49	12.915	1838	1841	1845	rVB2	56602	66154	3.77%	0.341%
50	13.004	1849	1856	1859	rBV	626189	627683	35.79%	3.239%
51	13.080	1865	1869	1873	rBV2	82126	144359	8.23%	0.745%
52	13.168	1881	1884	1885	rBV3	71316	75657	4.31%	0.390%
53	13.192	1885	1888	1891	rVB	187492	174356	9.94%	0.900%
54	13.227	1891	1894	1897	rBV2	46700	61543	3.51%	0.318%
55	13.257	1897	1899	1902	rVB	138060	102470	5.84%	0.529%
56	13.298	1902	1906	1909	rBV2	117749	130135	7.42%	0.672%
57	13.392	1919	1922	1924	rBV	71607	66312	3.78%	0.342%
58	13.421	1924	1927	1930	rBV	81850	87918	5.01%	0.454%
59	13.568	1949	1952	1954	rBV4	74850	95293	5.43%	0.492%
60	13.704	1972	1975	1979	rVB	70557	83791	4.78%	0.432%
61	13.809	1991	1993	1996	rBV2	63603	61428	3.50%	0.317%
62	13.839	1996	1998	2000	rBV	91981	98856	5.64%	0.510%
63	13.862	2000	2002	2004	rVV2	112203	119473	6.81%	0.617%
64	13.898	2005	2008	2010	rVV2	142535	195194	11.13%	1.007%
65	13.927	2010	2013	2019	rVB	357512	349275	19.92%	1.803%
66	14.062	2029	2036	2039	rBV2	1227872	1753797	100.00%	9.051%
67	14.092	2039	2041	2046	rVB	524468	482403	27.51%	2.490%
68	14.168	2052	2054	2057	rBV	171815	135733	7.74%	0.700%
69	14.215	2059	2062	2067	rVV4	108554	136370	7.78%	0.704%
70	14.451	2100	2102	2104	rVB	108439	75938	4.33%	0.392%
71	14.521	2111	2114	2116	rBV2	102573	91728	5.23%	0.473%
72	14.574	2121	2123	2125	rVV2	91899	75316	4.29%	0.389%
73	14.598	2125	2127	2129	rVB2	74741	58873	3.36%	0.304%
74	15.121	2211	2216	2219	rBV	575512	937666	53.46%	4.839%
75	15.227	2231	2234	2238	rBV	148239	192523	10.98%	0.994%
76	15.427	2265	2268	2275	rVB	347614	473820	27.02%	2.445%

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Misc :
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ClientSampleId : ETGI-332

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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77	15.498	2275	2280	2286	rBV	604716	862537	49.18%	4.451%
78	15.562	2286	2291	2294	rBV	777718	1038684	59.22%	5.360%
79	17.068	2542	2547	2555	rVB2	214647	406382	23.17%	2.097%
80	17.521	2621	2624	2632	rVB	166851	266140	15.18%	1.373%

Sum of corrected areas: 19377214

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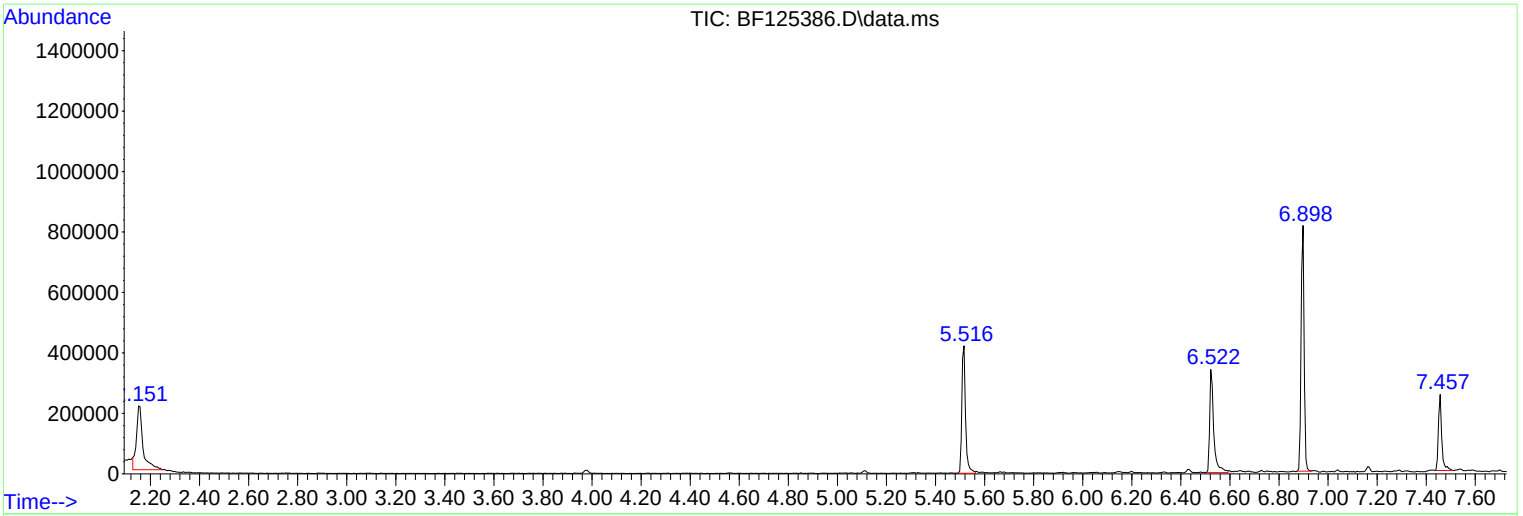
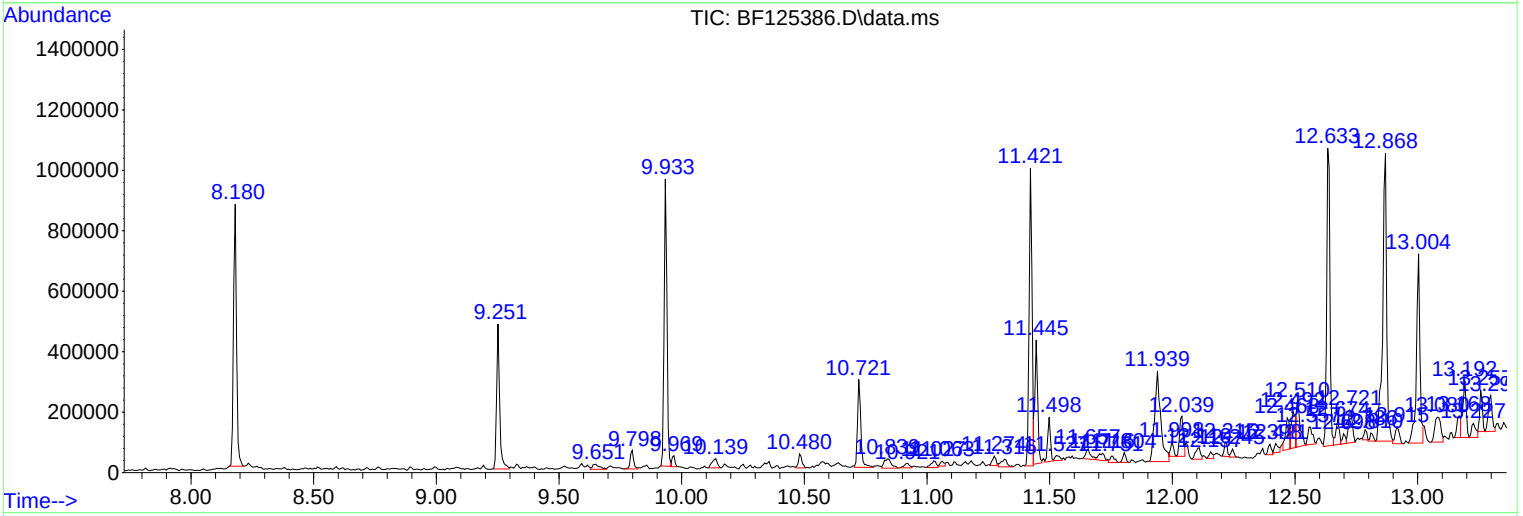
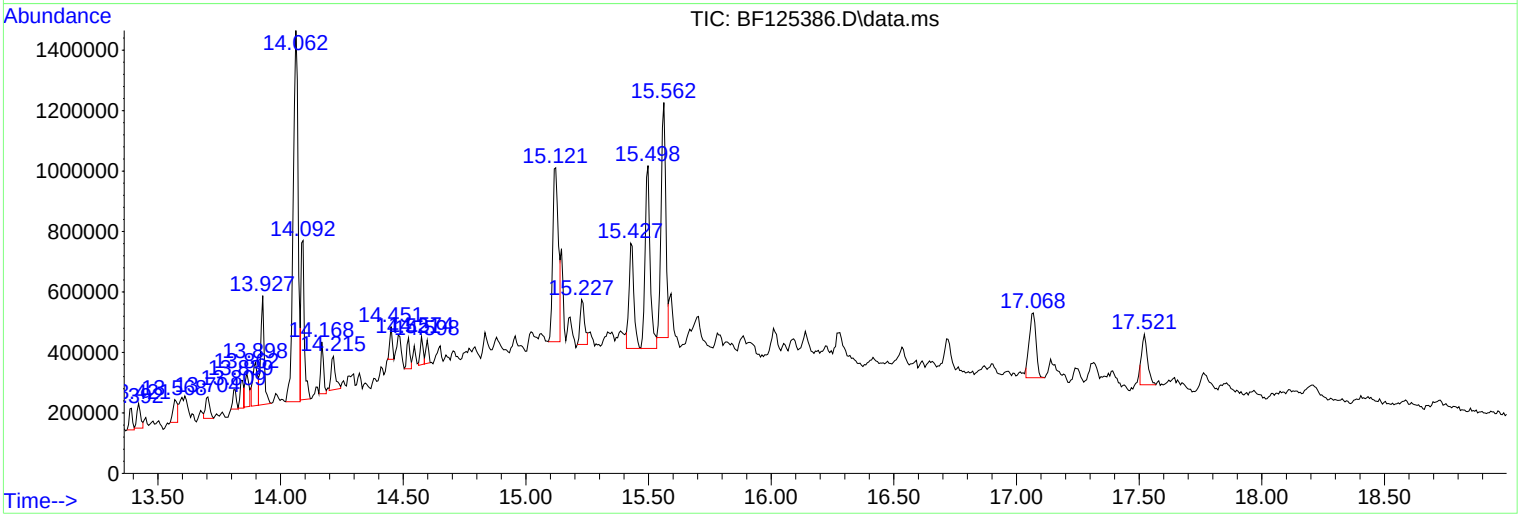
Instrument :
BNA_F
ClientSampleId :
ETGI-332

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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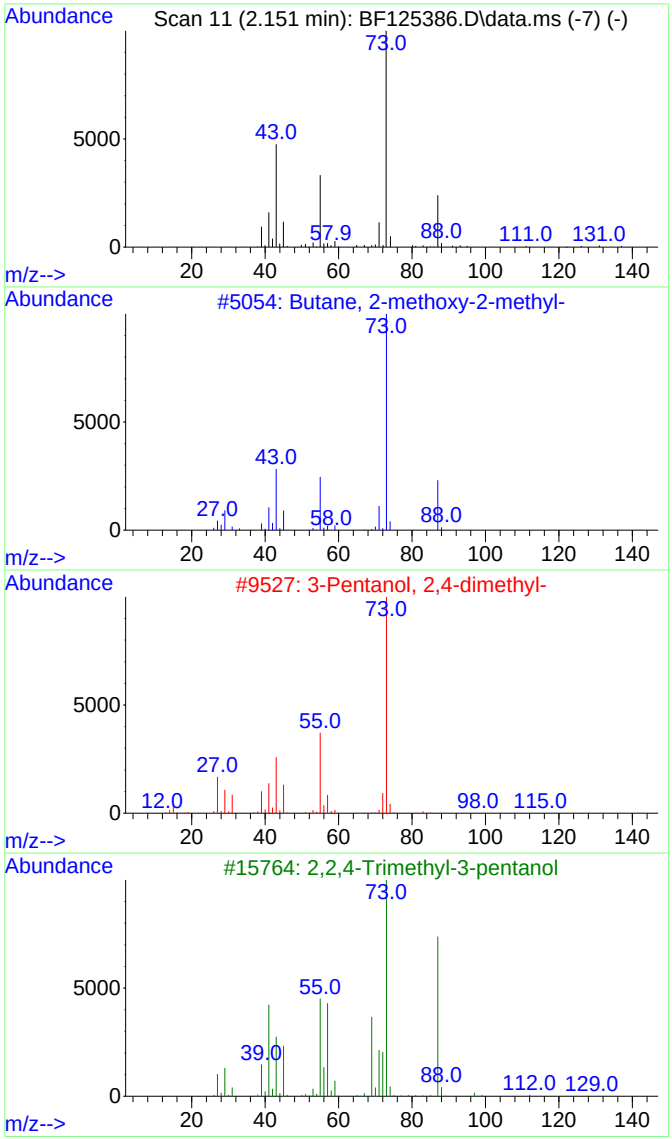
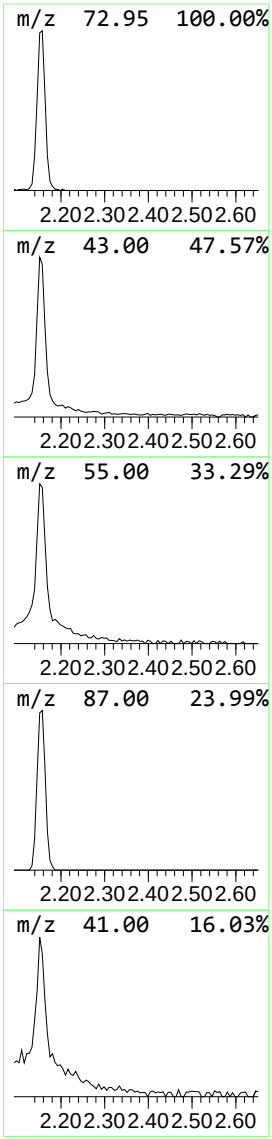
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.151	11.27 ng	390752	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	38
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35





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Sample : M3660-01 5X
Misc :
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Instrument : BNA_F
ClientSampleId : ETGI-332

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

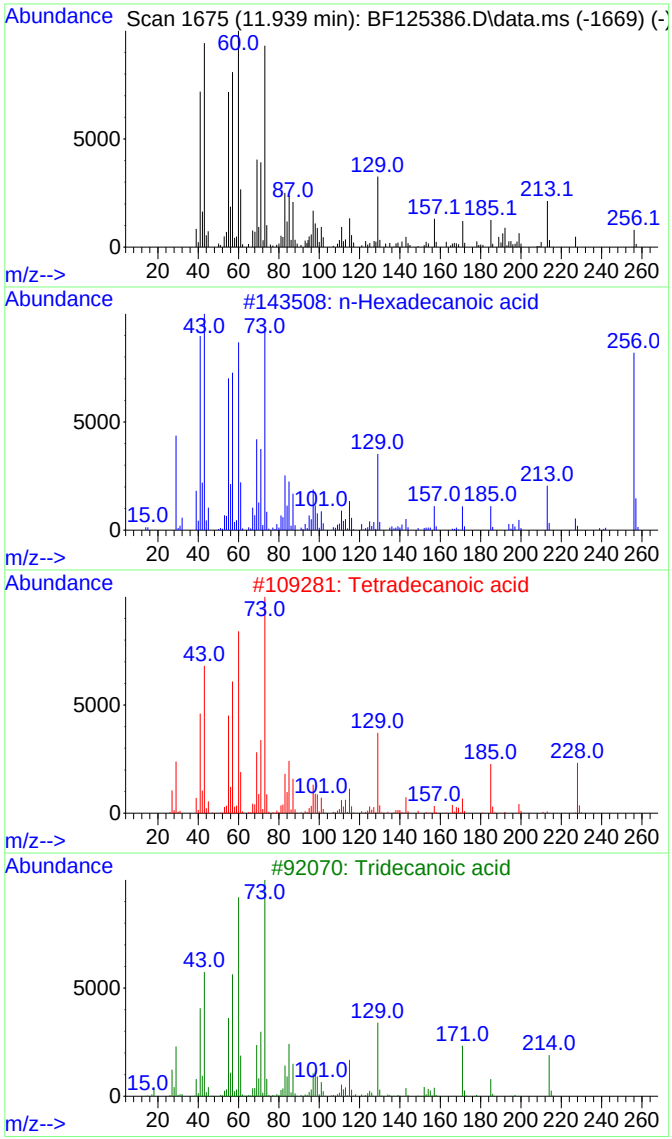
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

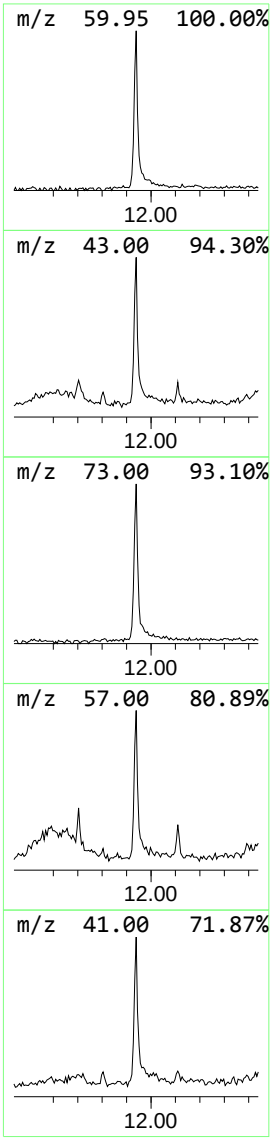
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	12.30 ng	507670	Phenanthrene-d10	11.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	76





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Instrument :
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ClientSampleId :
ETGI-332

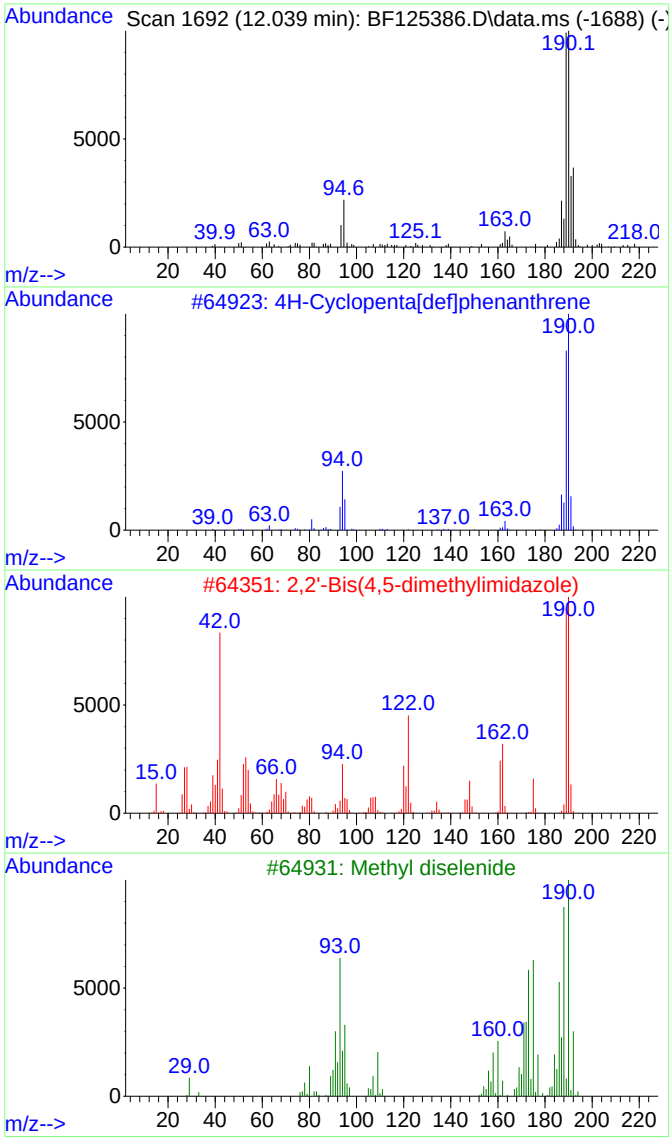
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

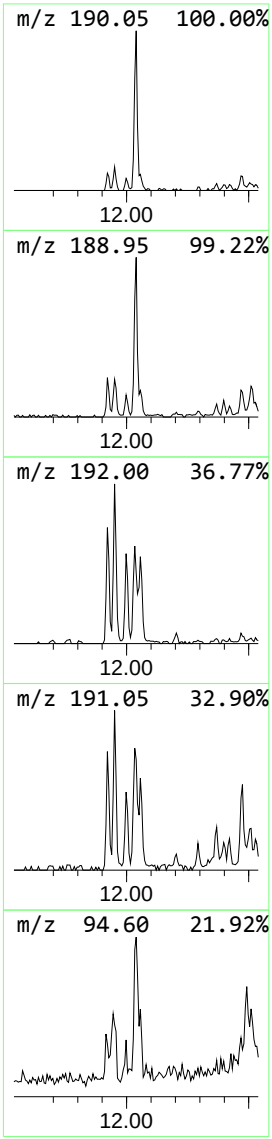
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.039	3.50 ng	144323	Phenanthrene-d10	11.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
3	Methyl diselenide	190	C2H6Se2	007101-31-7	43
4	Pyrimidine, 2-chloro-5-phenyl-	190	C10H7ClN2	022536-62-5	17
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	17





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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-332

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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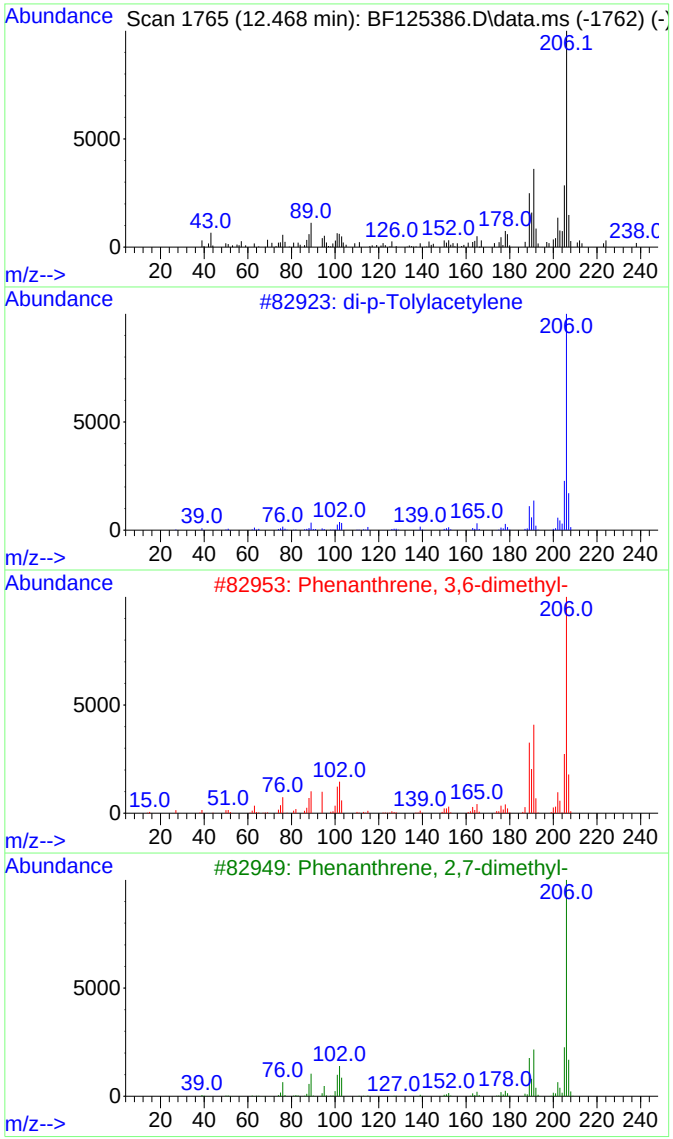
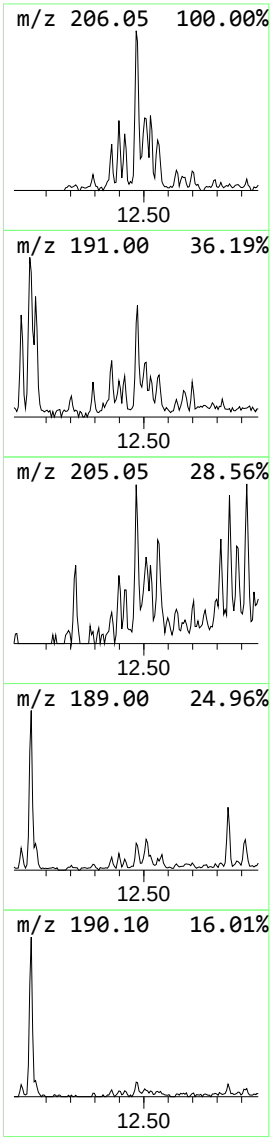
Peak Number 4 di-p-Tolylacetylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.468	3.07 ng	126634	Phenanthrene-d10	11.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	di-p-Tolylacetylene	206	C16H14	002789-88-0	94
2	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	93
3	Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	93
4	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	91
5	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	90





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Instrument : BNA_F
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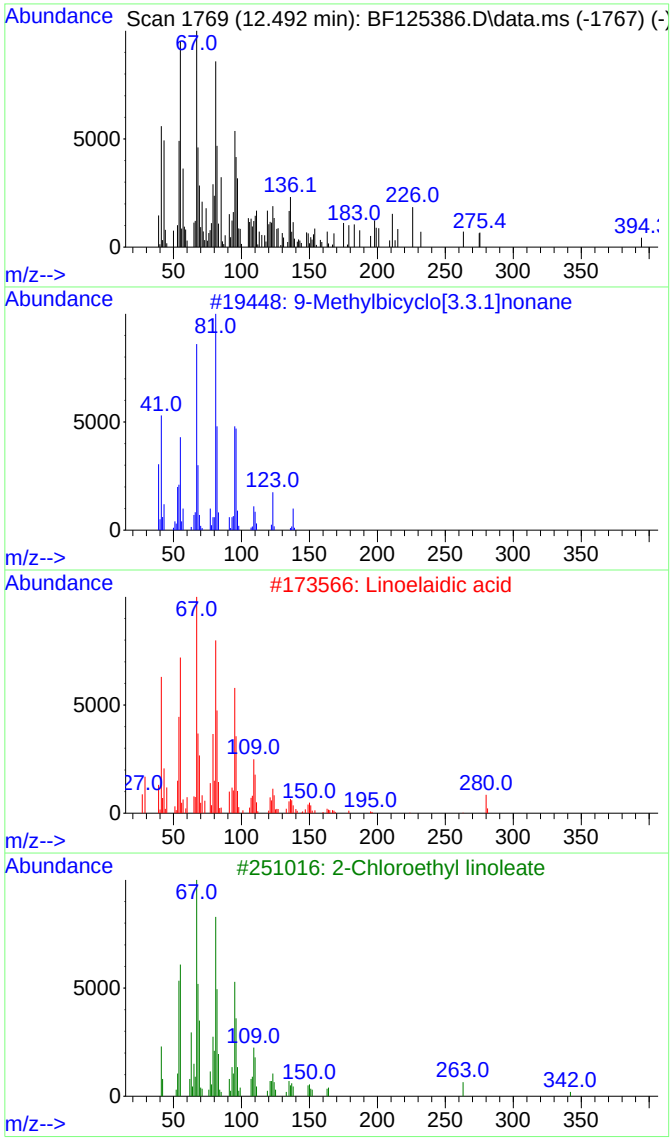
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

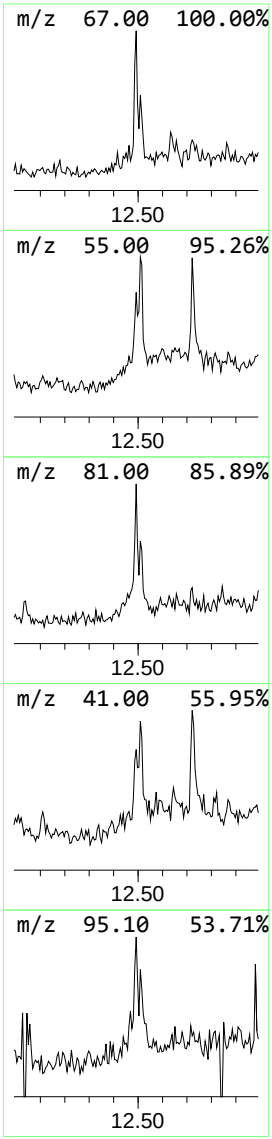
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9-Methylbicyclo[3.3.1]nonane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.492	3.58 ng	147632	Phenanthrene-d10	11.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Methylbicyclo[3.3.1]nonane	138	C10H18	025107-01-1	81
2	Linoelaidic acid	280	C18H32O2	000506-21-8	72
3	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	72
4	Cyclooctene, 3-methyl-	124	C9H16	013152-05-1	70
5	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	64





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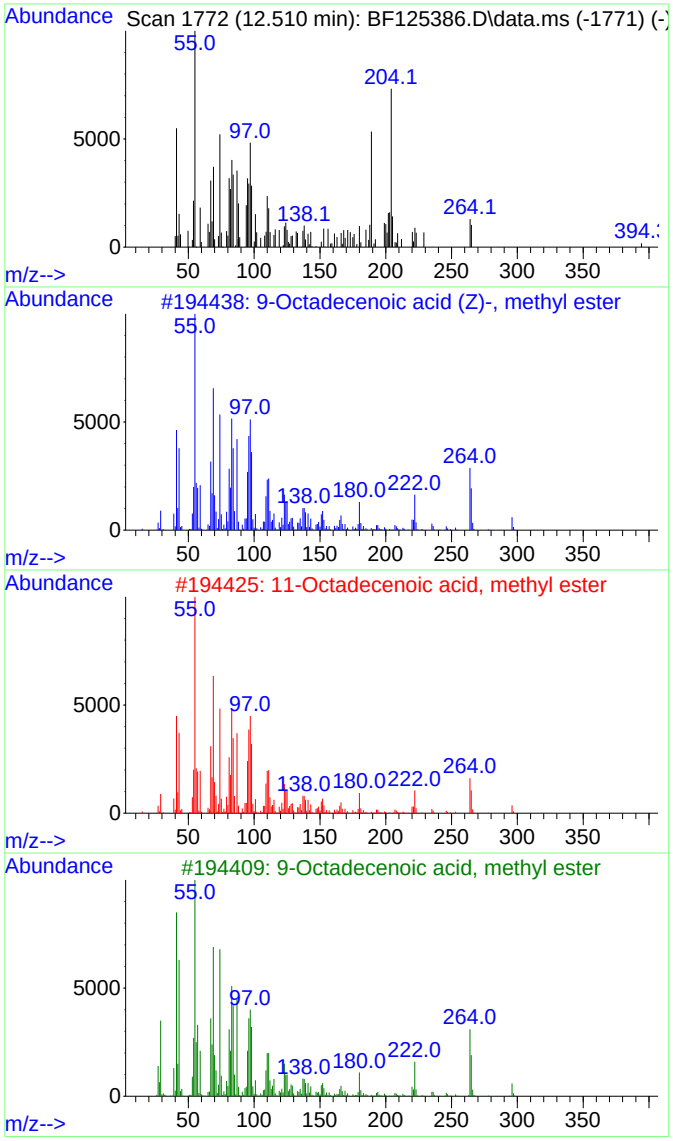
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

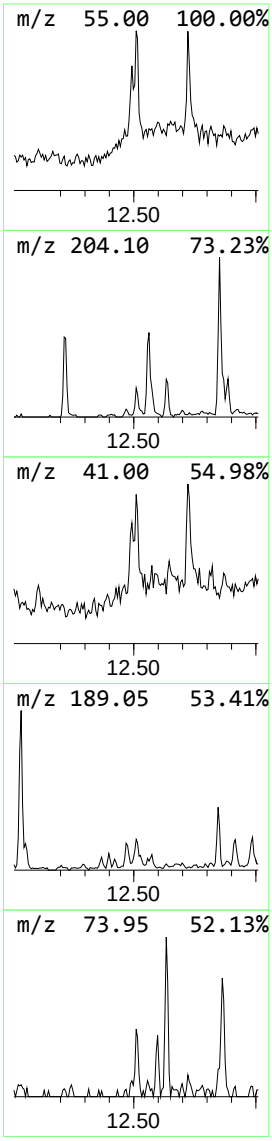
****

Peak Number 6 unknown12.510 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.510	3.53 ng	145605	Phenanthrene-d10	11.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	46
2	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	46
3	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	38
4	7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	38
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	38





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Acq On : 7 Sep 2021 14:15
Operator : JU/CG
Sample : M3660-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-332

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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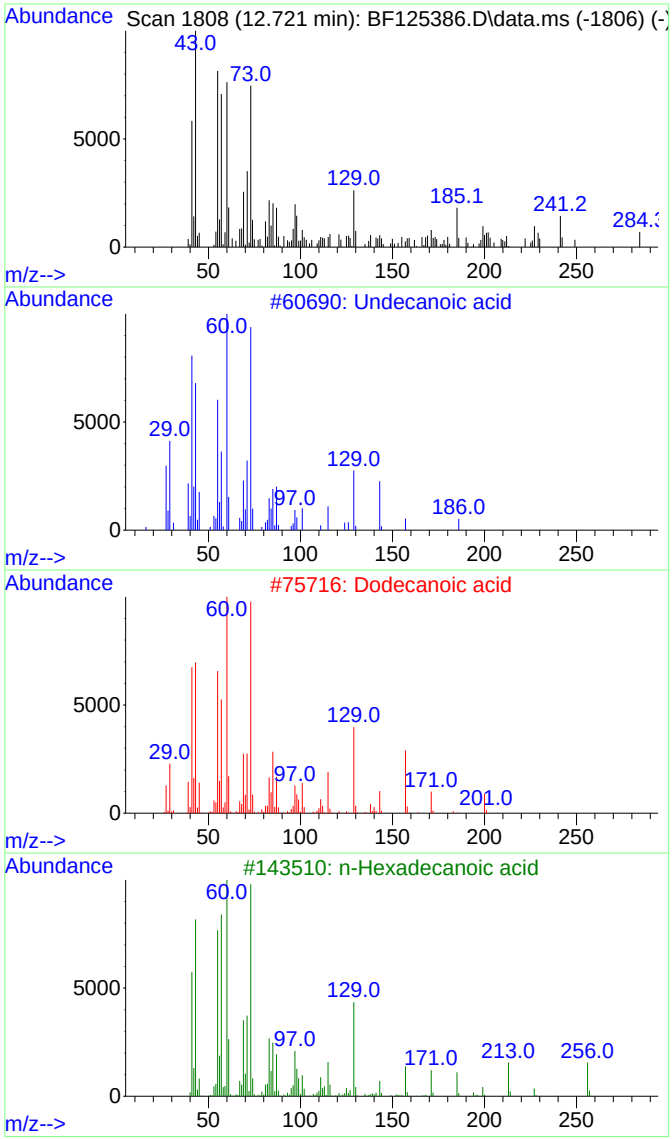
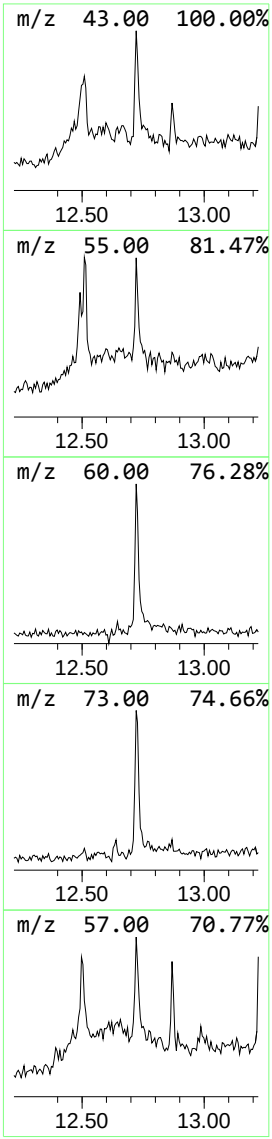
Peak Number 7 Undecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.721	2.96 ng	122312	Phenanthrene-d10	11.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	89
2	Dodecanoic acid	200	C12H24O2	000143-07-7	76
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	59





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Operator : JU/CG
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Misc :
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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TIC Library : C:\Database\NIST20.L
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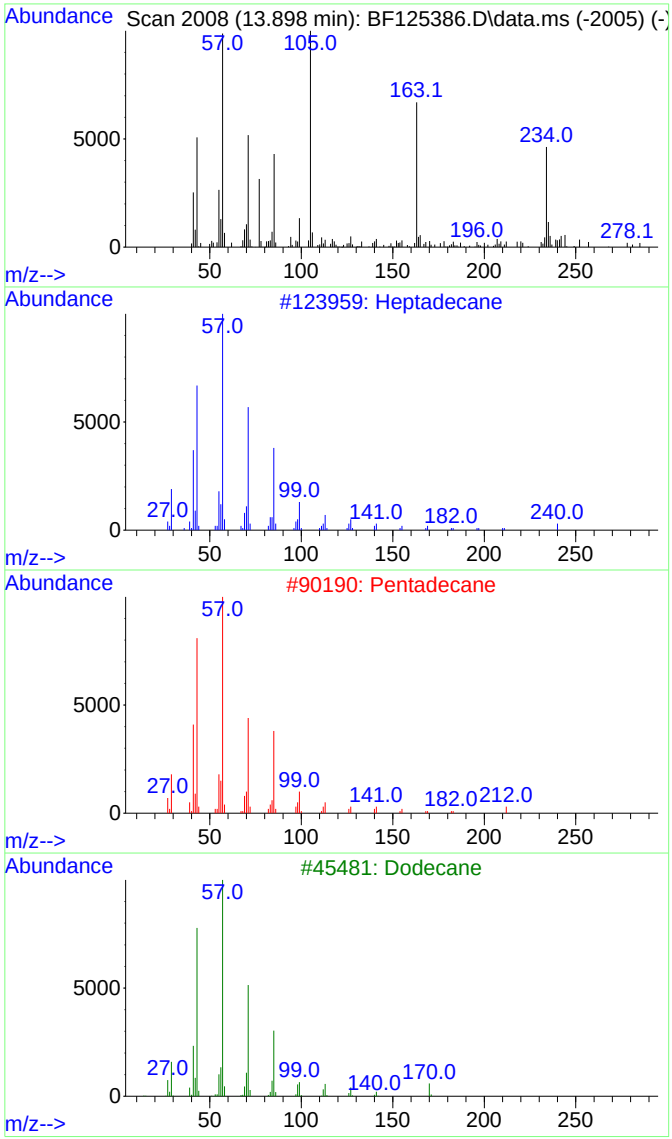
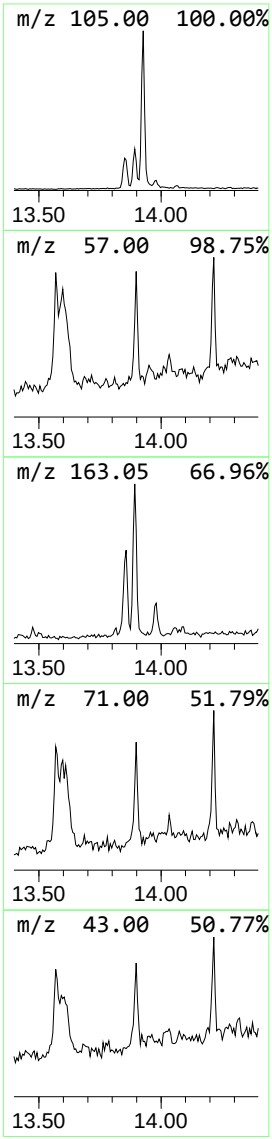
Peak Number 8 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	2.23 ng	195194	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	51
2	Pentadecane	212	C15H32	000629-62-9	49
3	Dodecane	170	C12H26	000112-40-3	25
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	25
5	Sulfurous acid, nonyl 2-propyl e...	250	C12H26O3S	1000309-12-0	25





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Operator : JU/CG
Sample : M3660-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-332

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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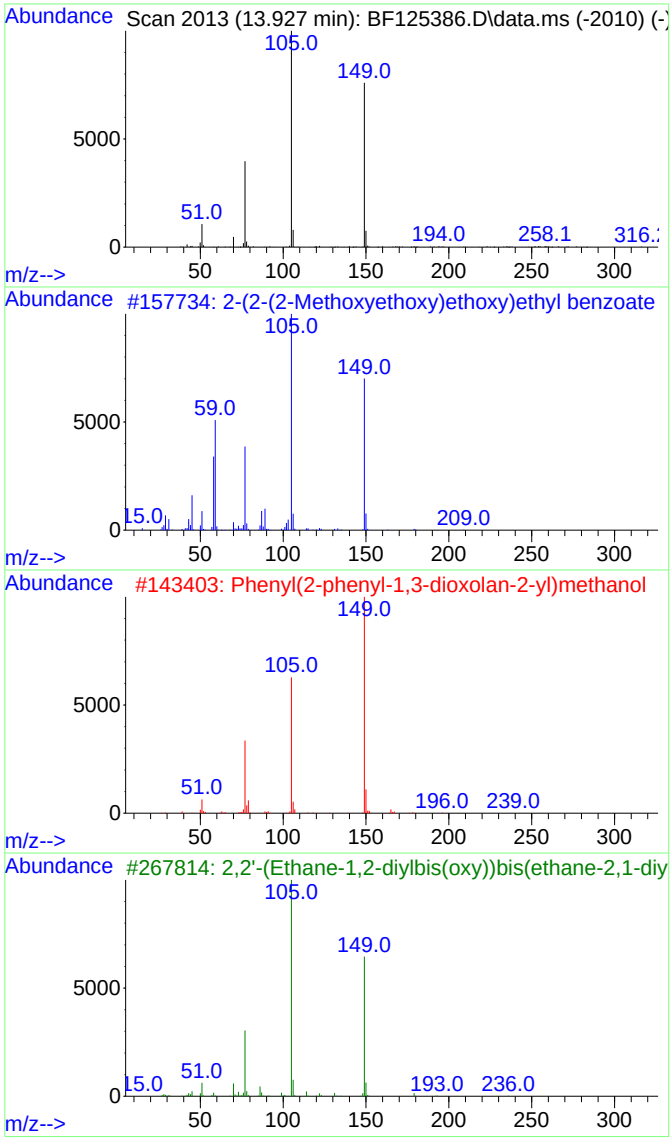
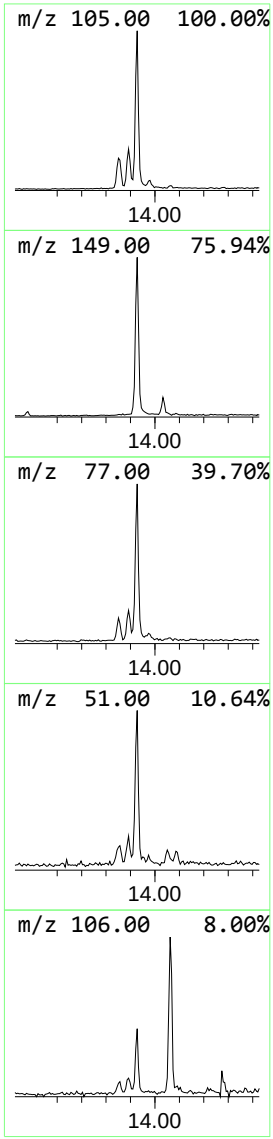
Peak Number 9 2-(2-(2-Methoxyethoxy)ethox... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	3.98 ng	349275	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	83
2	Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	78
3	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	64
4	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	52
5	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	43





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Operator : JU/CG
Sample : M3660-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ETGI-332

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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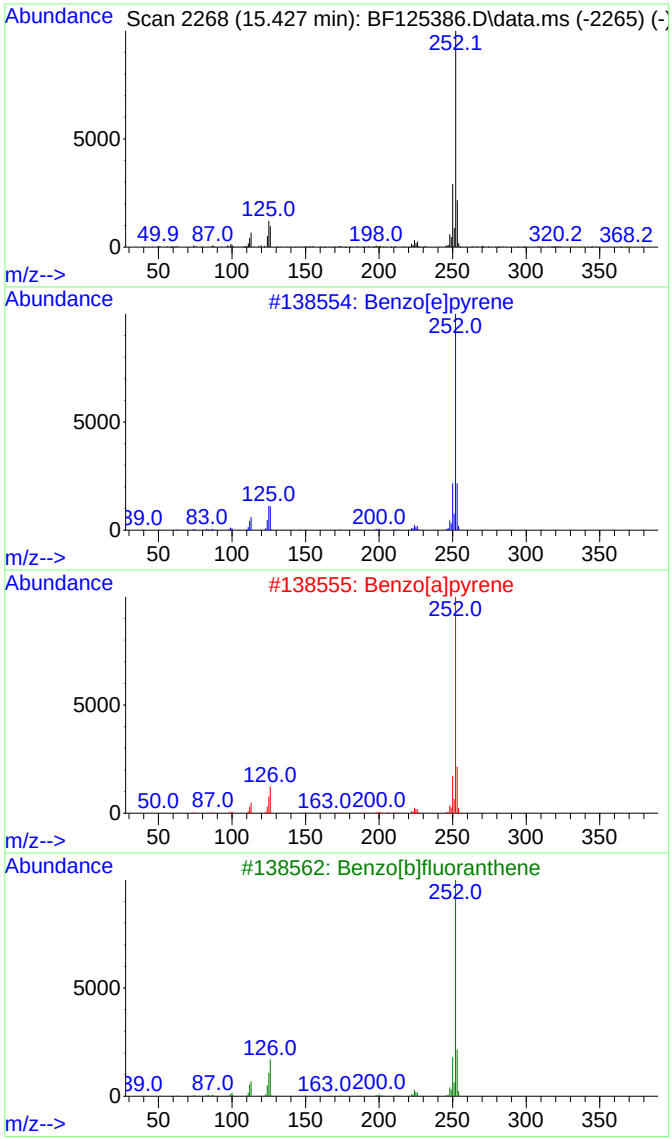
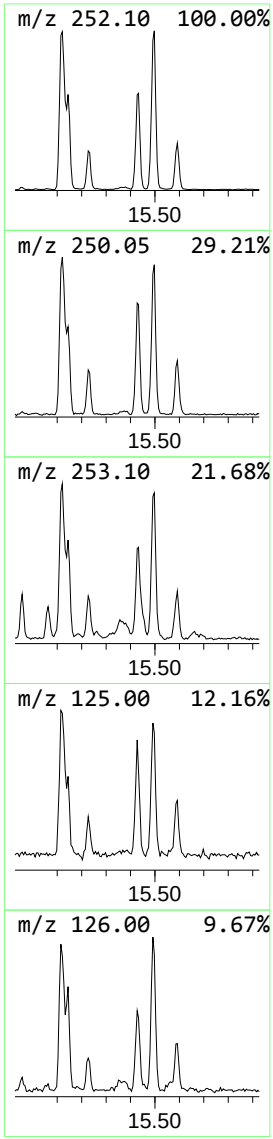
Peak Number 11 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.427	9.12 ng	473820	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[a]pyrene	252	C20H12	000050-32-8	95
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
4	Perylene	252	C20H12	000198-55-0	94
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94





Tentatively Identified Compound (LSC) summary

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Data File : BF125386.D
Acq On : 7 Sep 2021 14:15
Operator : JU/CG
Sample : M3660-01 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ETGI-332

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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...	2.151	11.3	ng	390752	1	6.898	693165	20.0
n-Hexadecanoic ...	11.939	12.3	ng	507670	4	11.421	825622	20.0
4H-Cyclopenta[d...	12.039	3.5	ng	144323	4	11.421	825622	20.0
di-p-Tolylacety...	12.468	3.1	ng	126634	4	11.421	825622	20.0
9-Methylbicyclo...	12.492	3.6	ng	147632	4	11.421	825622	20.0
unknown12.510	12.510	3.5	ng	145605	4	11.421	825622	20.0
Undecanoic acid	12.721	3.0	ng	122312	4	11.421	825622	20.0
Heptadecane	13.898	2.2	ng	195194	5	14.068	1753800	20.0
2-(2-(2-Methoxy...	13.927	4.0	ng	349275	5	14.068	1753800	20.0
Benzo[e]pyrene	15.427	9.1	ng	473820	6	15.562	1038680	20.0