LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125828.D
Acq On : 13 Oct 2021 15:49
Operator : JU/CG
Sample : M4047-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 149-ENV-1-GRAB

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-BF100721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125828.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	12	rVB	1298321	1514770	37.67%	3.989%
2	5.463	569	574	577	rBV	3682271	3371649	83.85%	8.878%
3	6.469	740	745	748	rBV	3444047	3329732	82.81%	8.767%
4	6.845	805	809	812	rBV	1236376	1046537	26.03%	2.756%
5	7.404	899	904	907	rBV	2317752	2138556	53.18%	5.631%
6	8.022	1006	1009	1022	rBV	710592	619913	15.42%	1.632%
7	8.122	1022	1026	1029	rBV	1751786	1420656	35.33%	3.741%
8	9.198	1205	1209	1212	rBV	4996216	4021001	100.00%	10.588%
9	9.316	1225	1229	1232	rBV	229270	191299	4.76%	0.504%
10	9.875	1321	1324	1327	rBV	1887439	1481213	36.84%	3.900%
11	9.910	1327	1330	1333	rVB	139483	123861	3.08%	0.326%
12	10.081	1354	1359	1362	rVB	50309	51041	1.27%	0.134%
13	10.422	1413	1417	1422	rVB	66486	58184	1.45%	0.153%
14	10.663	1454	1458	1461	rBV	2205237	1950181	48.50%	5.135%
15	11.357	1573	1576	1578	rBV	1427585	1211810	30.14%	3.191%
16	11.380	1578	1580	1584	rVV	819926	659869	16.41%	1.737%
17	11.433	1584	1589	1592	rVB	241150	220195	5.48%	0.580%
18	11.586	1609	1615	1618	rBV2	106855	113839	2.83%	0.300%
19	11.757	1641	1644	1650	rVB	99672	94468	2.35%	0.249%
20	11.857	1656	1661	1663	rBV	74503	74972	1.86%	0.197%
21	11.886	1663	1666	1670	rVV2	392037	333436	8.29%	0.878%
22	11.933	1670	1674	1677	rVB2	57775	78206	1.94%	0.206%
23	11.975	1677	1681	1683	rBV	120518	133897	3.33%	0.353%
24	12.157	1709	1712	1714	rBV	61031	55208	1.37%	0.145%
25	12.410	1751	1755	1758	rBV3	48310	58937	1.47%	0.155%
26	12.463	1758	1764	1767	rVV4	105943	132285	3.29%	0.348%
27	12.545	1775	1778	1779	rBV	68100	50462	1.25%	0.133%
28	12.569	1779	1782	1786	rVB	1142568	907699	22.57%	2.390%
29	12.669	1796	1799	1805	rBV3	130665	178095	4.43%	0.469%
30	12.798	1815	1821	1824	rBV	1005363	1065214	26.49%	2.805%
31	12.845	1827	1829	1835	rVB3	57594	70590	1.76%	0.186%
32	12.945	1842	1846	1849	rVV	3416463	2892351	71.93%	7.616%
33	13.016	1853	1858	1861	rBV2	58759	93016	2.31%	0.245%
34	13.104	1866	1873	1874	rBV4	66806	96247	2.39%	0.253%
35	13.127	1874	1877	1880	rVB2	139087	121187	3.01%	0.319%
36	13.192	1885	1888	1890	rVV	121832	96687	2.40%	0.255%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
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Acq On : 13 Oct 2021 15:49
Operator : JU/CG
Sample : M4047-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 149-ENV-1-GRAB

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-BF100721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.227	1890	1894	1897	rVB2	100104	106271	2.64%	0.280%
38	13.322	1908	1910	1913	rVB	59571	54547	1.36%	0.144%
39	13.351	1913	1915	1919	rBV2	54655	57413	1.43%	0.151%
40	13.627	1960	1962	1968	rVB2	53247	74866	1.86%	0.197%
41	13.745	1978	1982	1984	rBV2	65008	79469	1.98%	0.209%
42	13.774	1984	1987	1989	rVV	100009	99819	2.48%	0.263%
43	13.798	1989	1991	1995	rVV2	84176	117572	2.92%	0.310%
44	13.839	1995	1998	2006	rVB3	111785	161964	4.03%	0.426%
45	13.992	2019	2024	2027	rBV2	1435165	1822247	45.32%	4.798%
46	14.021	2027	2029	2035	rVB	615409	523688	13.02%	1.379%
47	14.098	2040	2042	2046	rVB	160061	131746	3.28%	0.347%
48	14.180	2051	2056	2059	rVV4	60100	84099	2.09%	0.221%
49	14.216	2059	2062	2066	rVB2	68372	82556	2.05%	0.217%
50	14.380	2086	2090	2093	rBV	117116	105412	2.62%	0.278%
51	14.416	2093	2096	2098	rVB	60327	53445	1.33%	0.141%
52	14.474	2102	2106	2108	rBV2	98237	116650	2.90%	0.307%
53	14.527	2113	2115	2118	rVB3	91711	84750	2.11%	0.223%
54	14.774	2153	2157	2159	rBV3	63556	80742	2.01%	0.213%
55	15.027	2196	2200	2203	rBV	525668	777975	19.35%	2.048%
56	15.133	2215	2218	2223	rVB	147636	157610	3.92%	0.415%
57	15.327	2247	2251	2256	rVB	334143	393400	9.78%	1.036%
58	15.386	2257	2261	2267	rVB	521280	621245	15.45%	1.636%
59	15.451	2267	2272	2275	rBV	807151	959471	23.86%	2.526%
60	15.480	2275	2277	2285	rVB2	177340	232868	5.79%	0.613%
61	15.921	2349	2352	2358	rVB2	52135	67721	1.68%	0.178%
62	16.892	2512	2517	2526	rVB2	202761	416533	10.36%	1.097%
63	17.074	2544	2548	2553	rBV	41885	64283	1.60%	0.169%
64	17.327	2586	2591	2603	rVB	148937	311320	7.74%	0.820%
65	17.557	2627	2630	2635	rVB	48255	81215	2.02%	0.214%

Sum of corrected areas: 37978160

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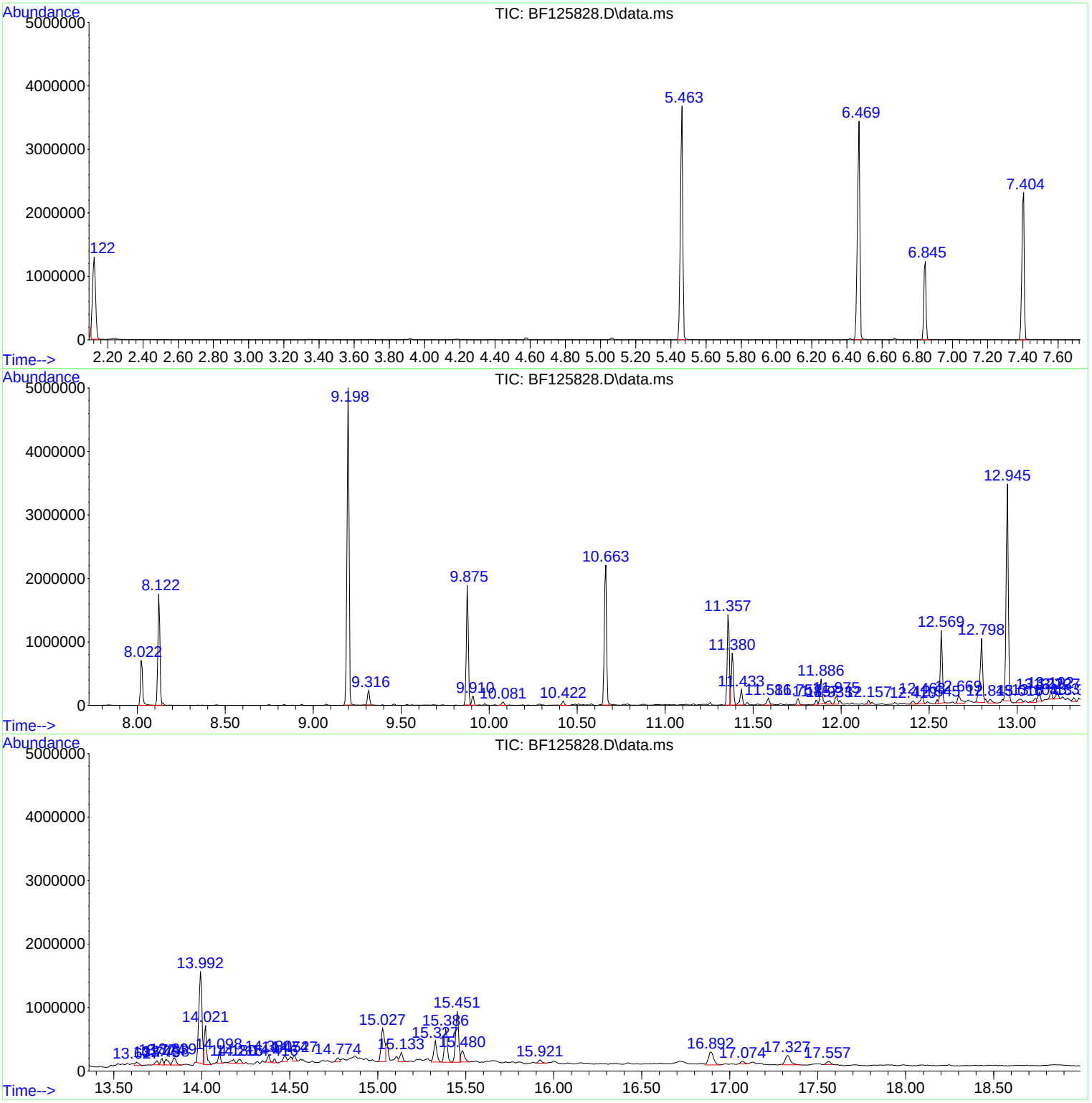
Instrument :
BNA_F
ClientSampleId :
149-ENV-1-GRAB

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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\BF101321\
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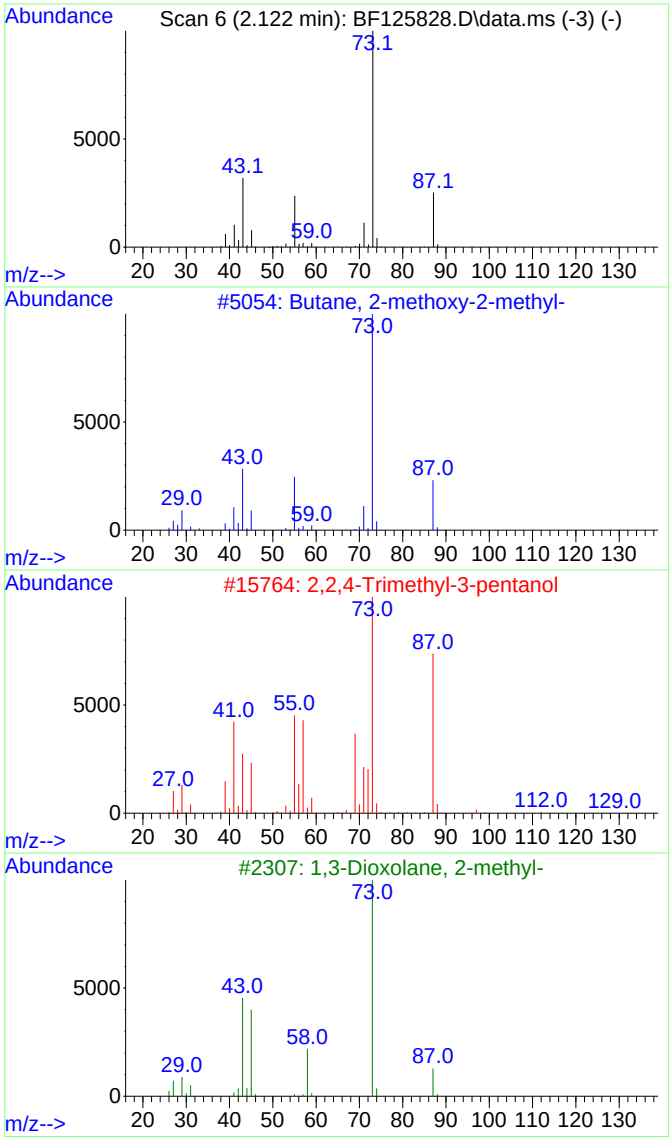
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

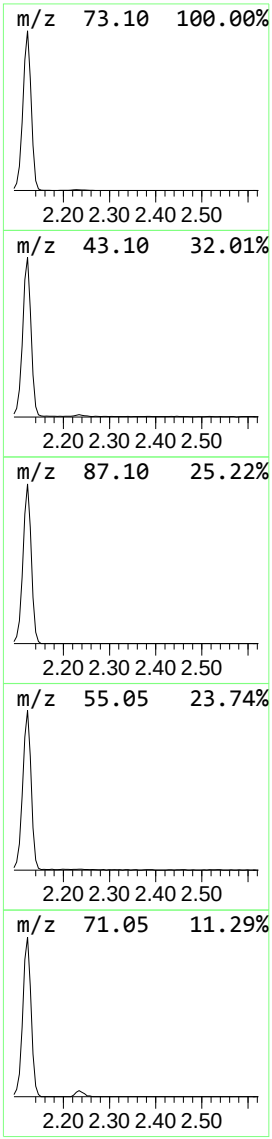
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	28.95 ng	1514770	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125828.D
Acq On : 13 Oct 2021 15:49
Operator : JU/CG
Sample : M4047-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 149-ENV-1-GRAB

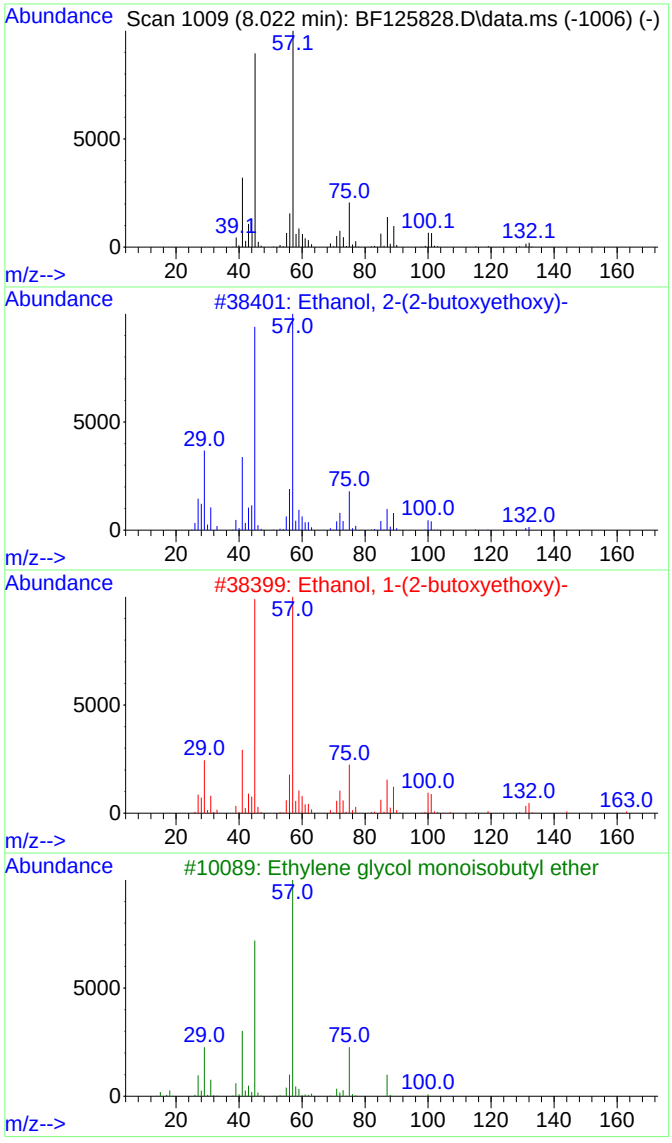
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

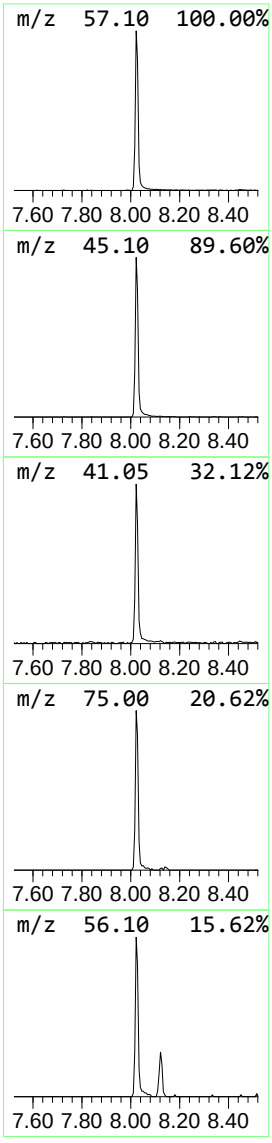
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.022	8.73 ng	619913	Naphthalene-d8	8.122

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	90
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
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Sample : M4047-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
149-ENV-1-GRAB

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
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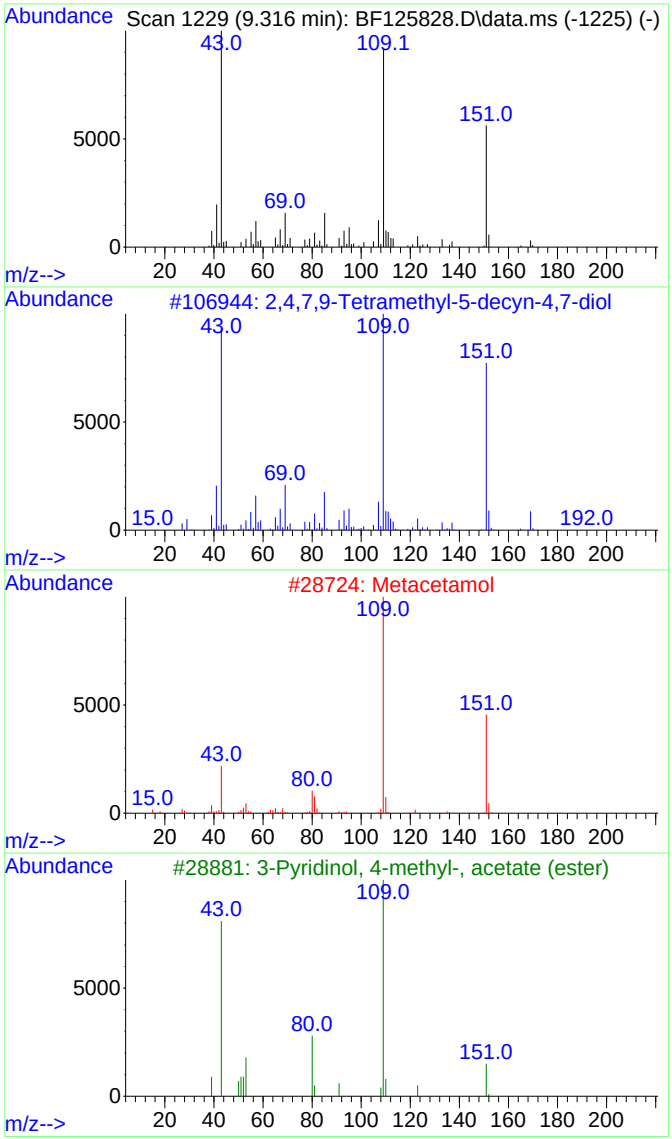
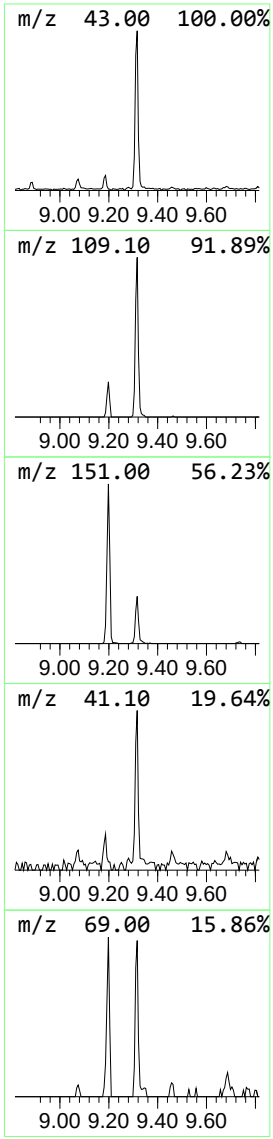
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.316	2.58 ng	191299	Acenaphthene-d10	9.875

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	53
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53
5	p-Isopropoxyaniline	151	C9H13NO	007664-66-6	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
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Sample : M4047-01
Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

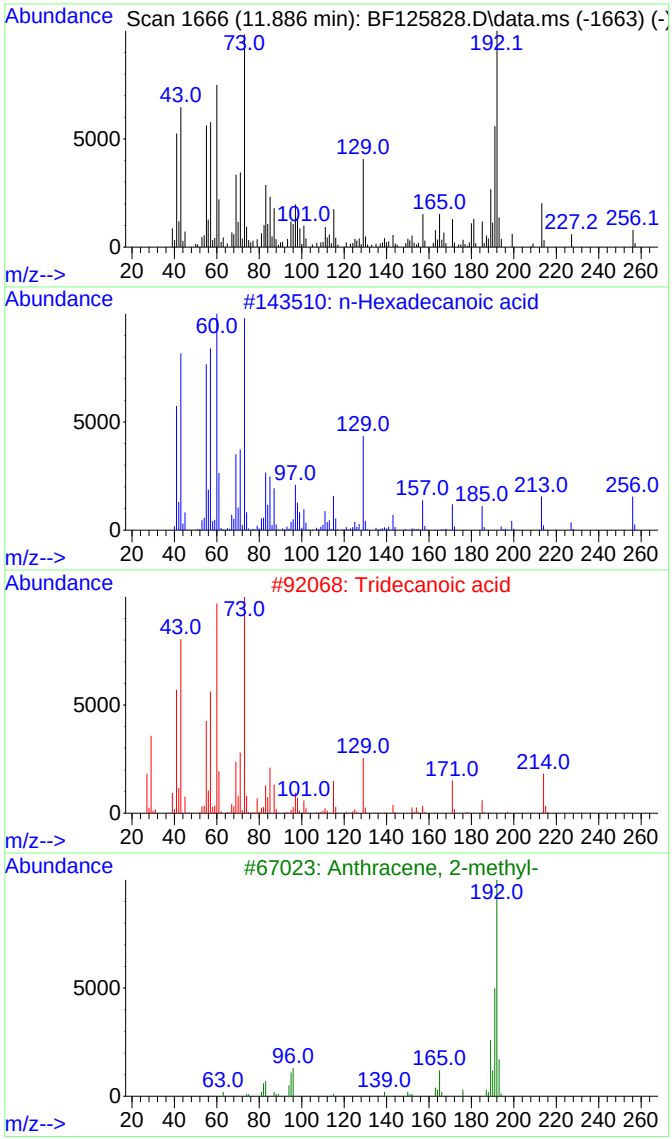
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

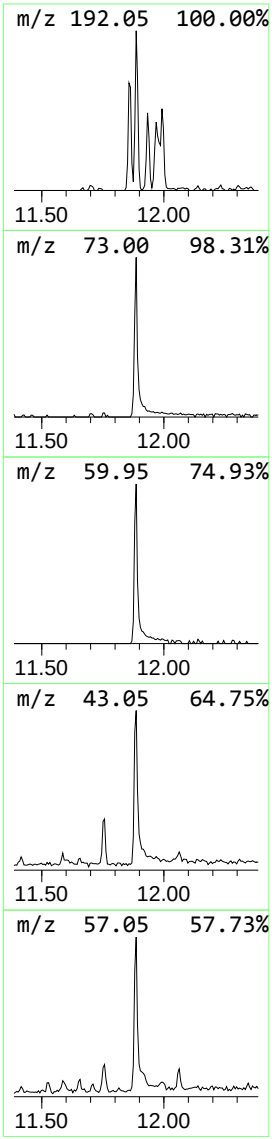
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	5.50 ng	333436	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	87
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	84
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	68
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
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Acq On : 13 Oct 2021 15:49
Operator : JU/CG
Sample : M4047-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
149-ENV-1-GRAB

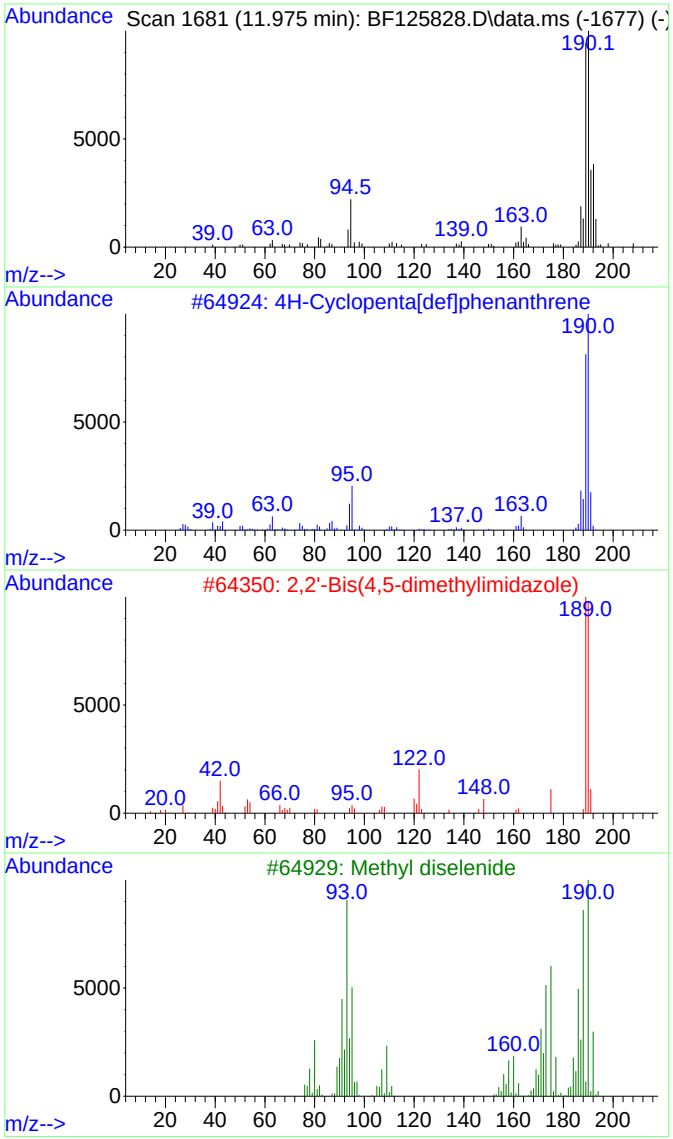
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

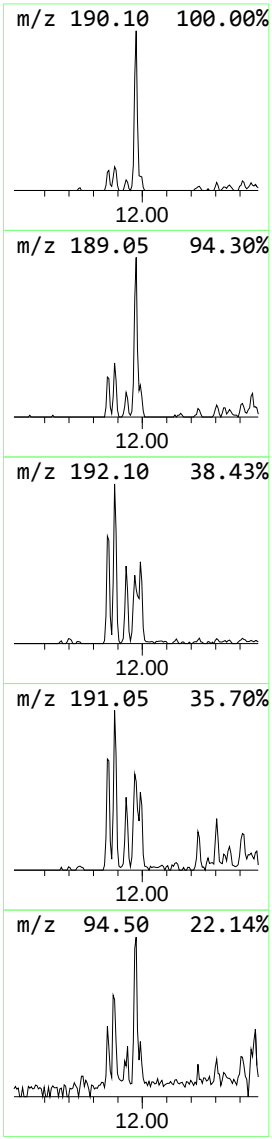
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.975	2.21 ng	133897	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	47
3	Methyl diselenide	190	C2H6Se2	007101-31-7	43
4	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	32
5	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	28





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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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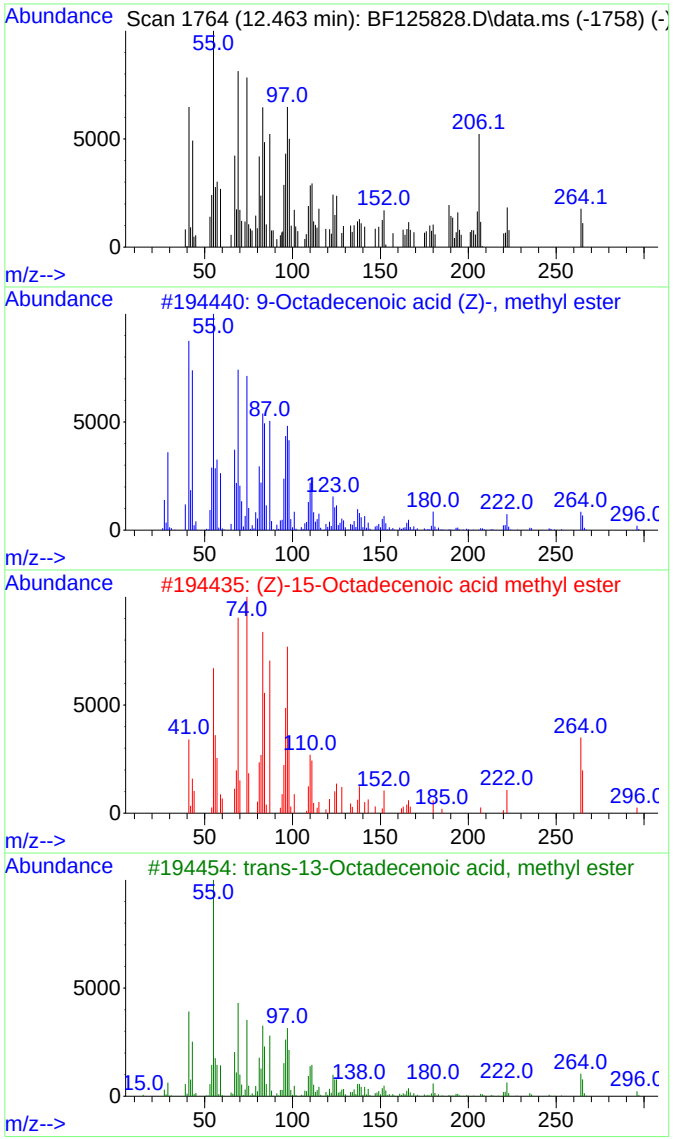
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

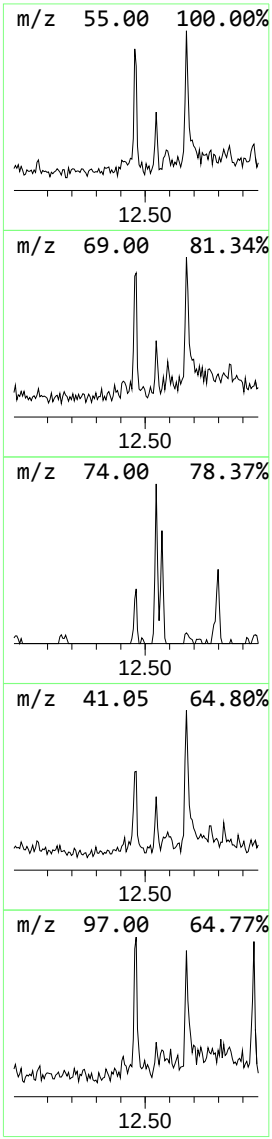
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.463	2.18 ng	132285	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
2	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	83
3	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	70
4	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	70
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125828.D
Acq On : 13 Oct 2021 15:49
Operator : JU/CG
Sample : M4047-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 149-ENV-1-GRAB

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

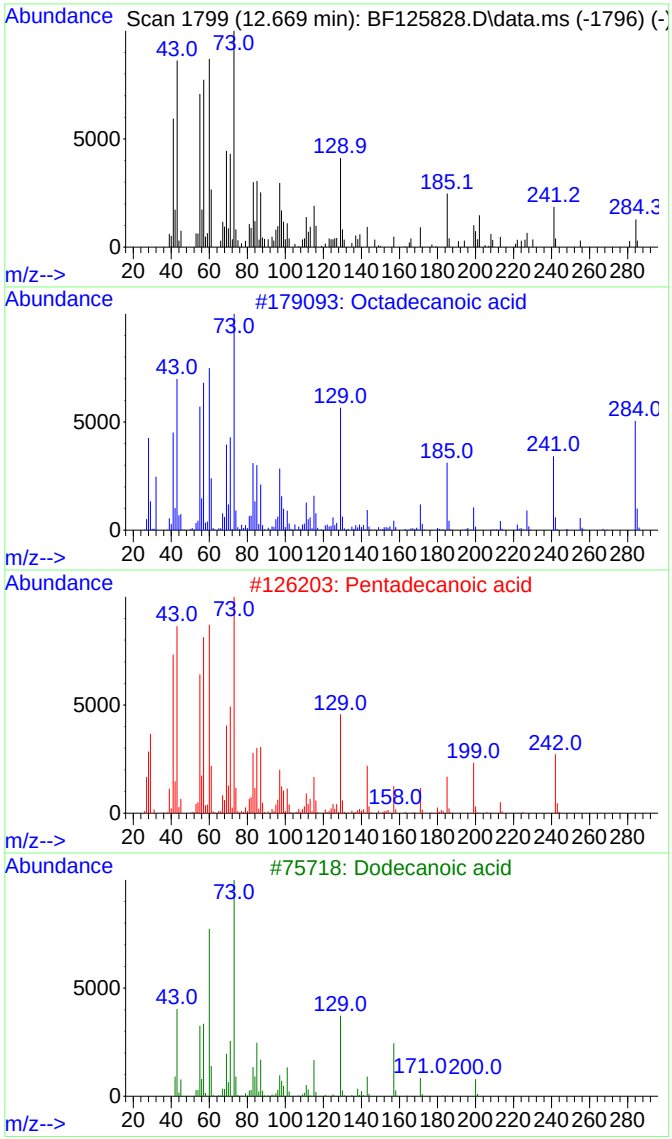
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

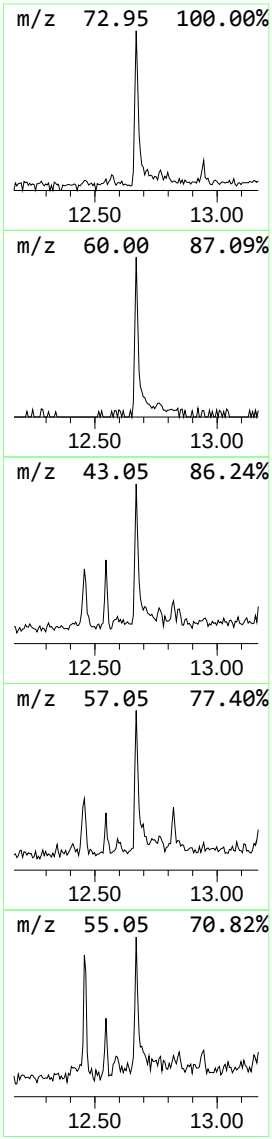
****

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.669	2.94 ng	178095	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Dodecanoic acid	200	C12H24O2	000143-07-7	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86





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Acq On : 13 Oct 2021 15:49
Operator : JU/CG
Sample : M4047-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 149-ENV-1-GRAB

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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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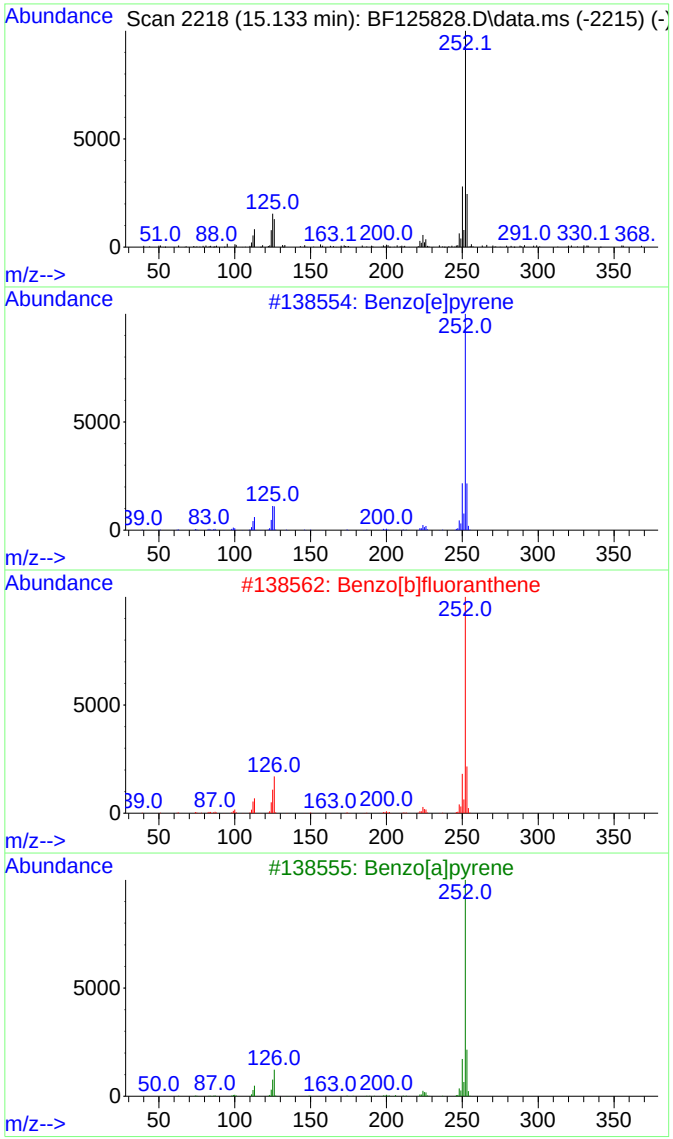
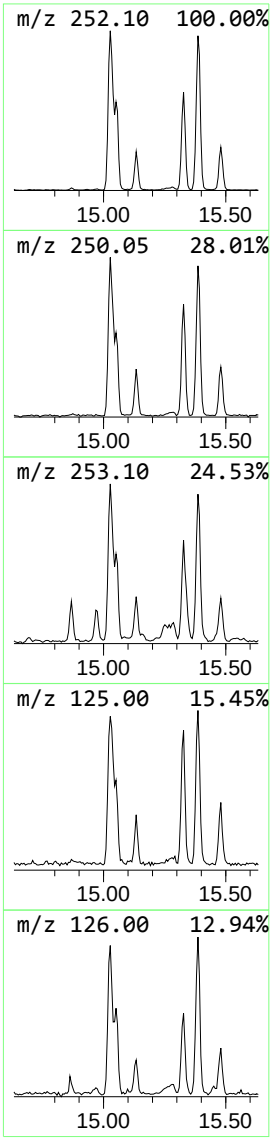
Peak Number 8 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	3.29 ng	157610	Perylene-d12	15.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
3	Benzo[a]pyrene	252	C20H12	000050-32-8	95
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90





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Data File : BF125828.D
Acq On : 13 Oct 2021 15:49
Operator : JU/CG
Sample : M4047-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
149-ENV-1-GRAB

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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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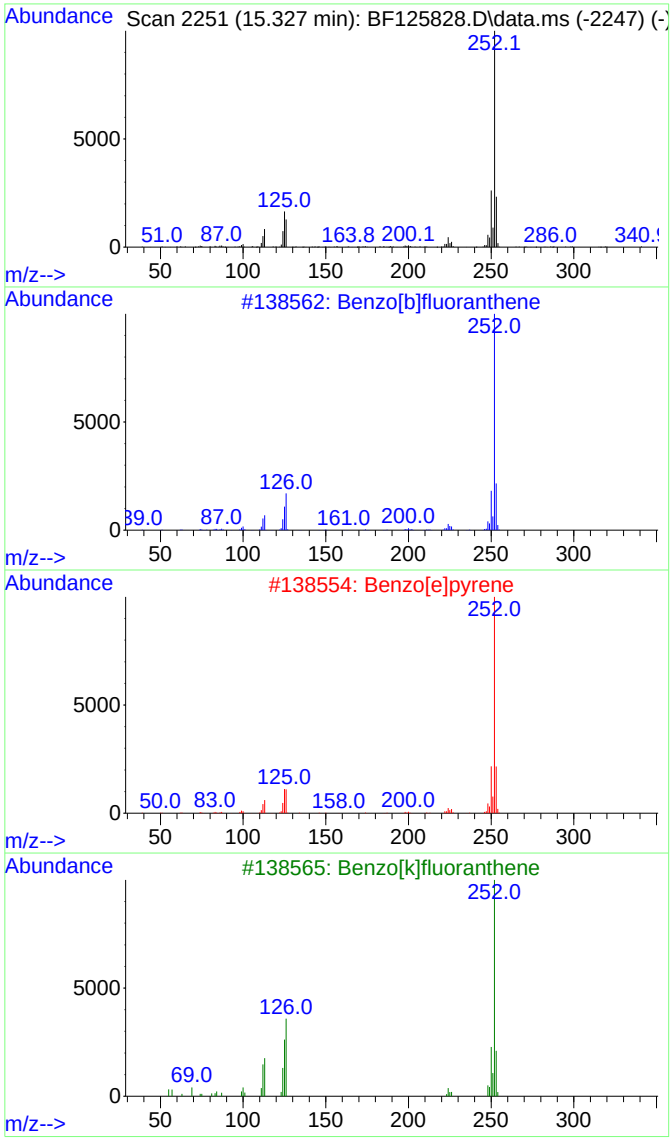
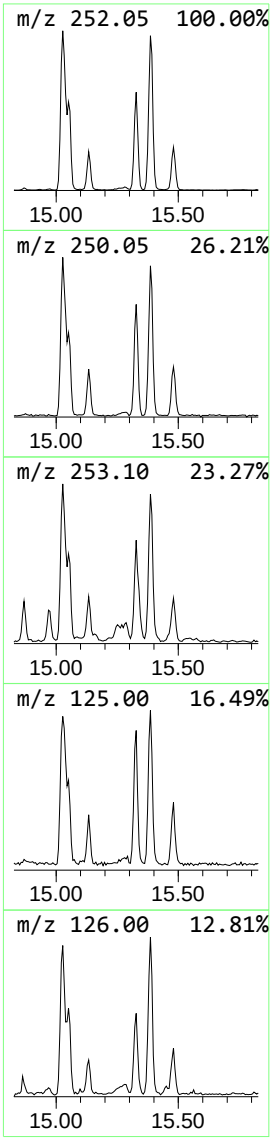
Peak Number 9 Benzo[j]fluoranthene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.327	8.20 ng	393400	Perylene-d12	15.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]fluoranthene	252	C20H12	000205-99-2	98
2	Benzo[e]pyrene	252	C20H12	000192-97-2	98
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
5	Benzo[a]pyrene	252	C20H12	000050-32-8	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125828.D
Acq On : 13 Oct 2021 15:49
Operator : JU/CG
Sample : M4047-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 149-ENV-1-GRAB

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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...	2.122	28.9	ng	1514770	1	6.845	1046540	20.0
Ethanol, 2-(2-b...	8.022	8.7	ng	619913	2	8.122	1420660	20.0
2,4,7,9-Tetrame...	9.316	2.6	ng	191299	3	9.875	1481210	20.0
n-Hexadecanoic ...	11.886	5.5	ng	333436	4	11.357	1211810	20.0
4H-Cyclopenta[d...	11.975	2.2	ng	133897	4	11.357	1211810	20.0
9-Octadecenoic ...	12.463	2.2	ng	132285	4	11.357	1211810	20.0
Octadecanoic acid	12.669	2.9	ng	178095	4	11.357	1211810	20.0
Benzo[e]pyrene	15.133	3.3	ng	157610	6	15.451	959471	20.0
Benzo[j]fluoran...	15.327	8.2	ng	393400	6	15.451	959471	20.0