LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101023\
Data File : BF135696.D
Acq On : 10 Oct 2023 21:09
Operator : CG\JU
Sample : 04753-01
Misc :
ALS Vial : 16 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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135696.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	14	17	25	rVB	25213	35342	1.38%	0.129%
2	2.775	112	117	126	rVB	37829	65592	2.56%	0.239%
3	4.334	379	382	391	rBV	79773	132197	5.16%	0.482%
4	4.975	484	491	509	rBV	1666866	2481838	96.92%	9.049%
5	5.381	556	560	585	rBV	2408256	2550614	99.60%	9.300%
6	5.763	620	625	630	rBV	64234	67531	2.64%	0.246%
7	6.392	728	732	744	rBV	2334933	2487989	97.16%	9.071%
8	6.739	788	791	804	rVB	698655	632960	24.72%	2.308%
9	7.304	883	887	902	rBV	1667930	1655508	64.65%	6.036%
10	8.016	1005	1008	1025	rVB	917927	833466	32.55%	3.039%
11	9.092	1187	1191	1195	rBV	2625607	2560836	100.00%	9.337%
12	9.216	1207	1212	1222	rVB	390837	416217	16.25%	1.518%
13	9.433	1245	1249	1252	rBV	21423	26068	1.02%	0.095%
14	9.639	1279	1284	1287	rBV2	31884	33605	1.31%	0.123%
15	9.774	1303	1307	1310	rBV	1010596	834086	32.57%	3.041%
16	9.804	1310	1312	1321	rVB2	68516	76751	3.00%	0.280%
17	9.986	1339	1343	1347	rVB2	26473	28187	1.10%	0.103%
18	10.327	1398	1401	1406	rVB	92808	82579	3.22%	0.301%
19	10.569	1439	1442	1458	rBV	1596841	1640558	64.06%	5.981%
20	10.692	1458	1463	1466	rVV4	34927	43278	1.69%	0.158%
21	10.880	1488	1495	1497	rBV3	34405	47369	1.85%	0.173%
22	11.169	1539	1544	1548	rVB2	53656	63119	2.46%	0.230%
23	11.269	1557	1561	1563	rBV	1036141	866491	33.84%	3.159%
24	11.292	1563	1565	1570	rVV	645085	542905	21.20%	1.979%
25	11.351	1571	1575	1578	rVB	75274	75030	2.93%	0.274%
26	11.516	1599	1603	1608	rBV2	63360	75887	2.96%	0.277%
27	11.604	1614	1618	1621	rBV	34088	36427	1.42%	0.133%
28	11.686	1630	1632	1637	rVB3	20888	25786	1.01%	0.094%
29	11.774	1644	1647	1650	rBV	113267	100952	3.94%	0.368%
30	11.804	1650	1652	1659	rVV	347578	355581	13.89%	1.296%
31	11.886	1663	1666	1669	rVV	200300	203757	7.96%	0.743%
32	11.910	1669	1670	1674	rVB	81059	56893	2.22%	0.207%
33	12.074	1695	1698	1700	rBV2	57075	50859	1.99%	0.185%
34	12.116	1702	1705	1709	rVB2	66185	59224	2.31%	0.216%
35	12.257	1726	1729	1732	rBV2	34053	31045	1.21%	0.113%
36	12.327	1738	1741	1744	rBV	90534	87214	3.41%	0.318%

LSC Area Percent Report

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Data File : BF135696.D
Acq On : 10 Oct 2023 21:09
Operator : CG\JU
Sample : 04753-01
Misc :
ALS Vial : 16 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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.368	1744	1748	1753	rVB5	68599	105986	4.14%	0.386%
38	12.427	1753	1758	1765	rVB5	41312	78927	3.08%	0.288%
39	12.492	1765	1769	1773	rBV	874502	749613	29.27%	2.733%
40	12.592	1784	1786	1792	rBV5	54359	66799	2.61%	0.244%
41	12.645	1792	1795	1798	rVV	67934	64610	2.52%	0.236%
42	12.721	1802	1808	1814	rVV	722236	765597	29.90%	2.791%
43	12.780	1815	1818	1822	rVB3	43110	48648	1.90%	0.177%
44	12.868	1828	1833	1836	rBV	2247589	2153870	84.11%	7.853%
45	12.951	1842	1847	1851	rBV2	50478	90023	3.52%	0.328%
46	13.033	1858	1861	1863	rBV3	44322	58610	2.29%	0.214%
47	13.057	1863	1865	1868	rVB	118418	99486	3.88%	0.363%
48	13.098	1868	1872	1874	rBV3	27295	29983	1.17%	0.109%
49	13.121	1874	1876	1879	rVB	93689	73683	2.88%	0.269%
50	13.163	1879	1883	1887	rBV2	73076	80141	3.13%	0.292%
51	13.251	1895	1898	1901	rBV	51959	49534	1.93%	0.181%
52	13.286	1901	1904	1907	rBV	53265	52358	2.04%	0.191%
53	13.439	1926	1930	1932	rBV3	36106	37933	1.48%	0.138%
54	13.580	1951	1954	1957	rVB3	24771	29520	1.15%	0.108%
55	13.686	1966	1972	1974	rBV2	52419	73700	2.88%	0.269%
56	13.704	1974	1975	1978	rVV2	43848	32692	1.28%	0.119%
57	13.733	1978	1980	1983	rVV	34151	38867	1.52%	0.142%
58	13.768	1983	1986	1988	rVV3	45315	49077	1.92%	0.179%
59	13.792	1988	1990	1996	rVB3	25151	39294	1.53%	0.143%
60	13.857	1996	2001	2003	rBV2	41698	65152	2.54%	0.238%
61	13.933	2007	2014	2017	rVV2	624290	862571	33.68%	3.145%
62	13.957	2017	2018	2025	rVB	230994	203689	7.95%	0.743%
63	14.039	2030	2032	2036	rVB	40542	33348	1.30%	0.122%
64	14.092	2037	2041	2048	rBV4	36431	65406	2.55%	0.238%
65	14.327	2076	2081	2084	rBV	52836	64230	2.51%	0.234%
66	14.362	2084	2087	2090	rVV3	30191	29833	1.16%	0.109%
67	14.398	2090	2093	2096	rVV2	50550	62164	2.43%	0.227%
68	14.457	2100	2103	2108	rVB3	51388	76773	3.00%	0.280%
69	14.827	2162	2166	2170	rBV6	19983	28323	1.11%	0.103%
70	14.980	2188	2192	2195	rBV	172195	234533	9.16%	0.855%
71	15.033	2199	2201	2208	rVB3	56045	66963	2.61%	0.244%
72	15.092	2208	2211	2217	rBV	34967	48107	1.88%	0.175%
73	15.280	2239	2243	2250	rVB	114873	130361	5.09%	0.475%
74	15.345	2250	2254	2260	rBV	159724	186275	7.27%	0.679%
75	15.404	2260	2264	2268	rBV	449698	529353	20.67%	1.930%
76	15.586	2291	2295	2299	rBV6	17486	32602	1.27%	0.119%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101023\
Data File : BF135696.D
Acq On : 10 Oct 2023 21:09
Operator : CG\JU
Sample : 04753-01
Misc :
ALS Vial : 16 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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	15.845	2334	2339	2345	rBV5	26173	50176	1.96%	0.183%
78	15.980	2358	2362	2368	rVB2	21456	38123	1.49%	0.139%
79	16.598	2463	2467	2474	rVB5	22830	41200	1.61%	0.150%
80	16.909	2512	2520	2532	rBV	68270	173866	6.79%	0.634%
81	17.362	2591	2597	2608	rVB2	54506	116412	4.55%	0.424%
82	17.633	2637	2643	2649	rBV6	22236	55145	2.15%	0.201%

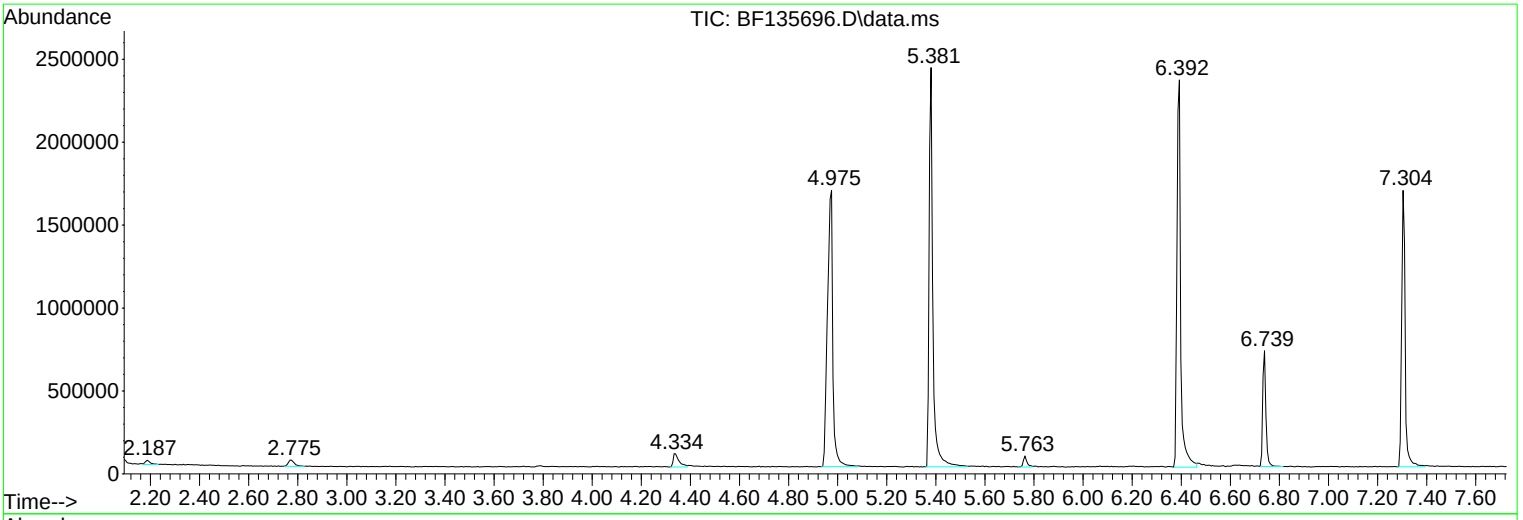
Sum of corrected areas: 27427297

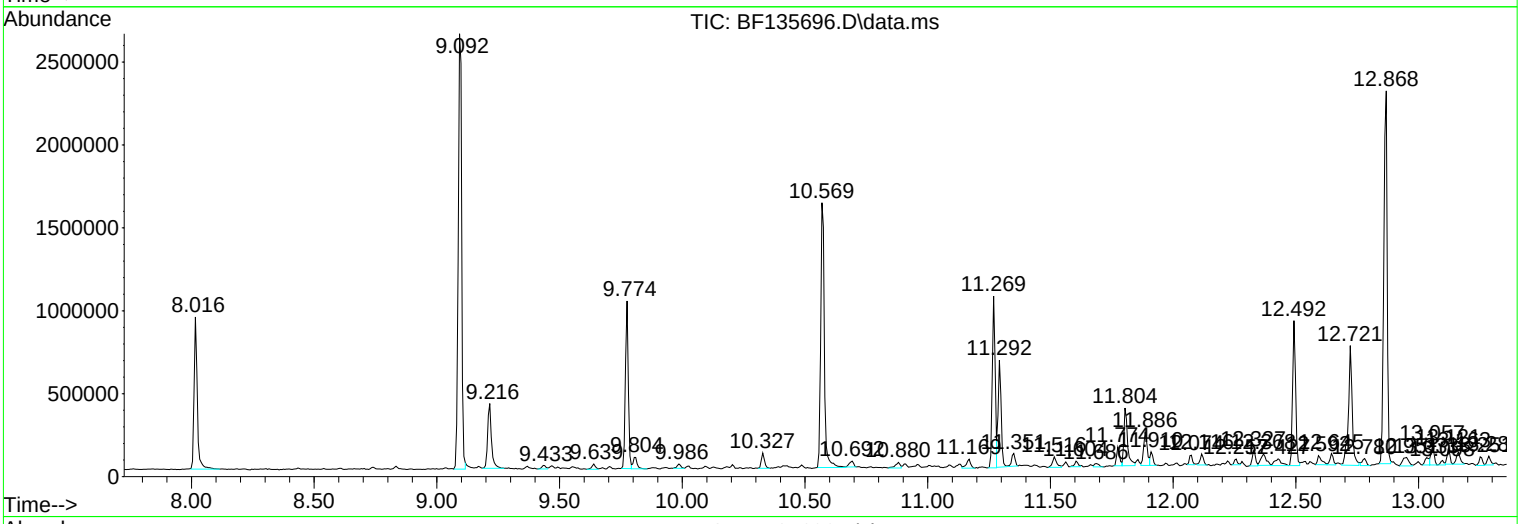
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101023\
Data File : BF135696.D
Acq On : 10 Oct 2023 21:09
Operator : CG\JU
Sample : 04753-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

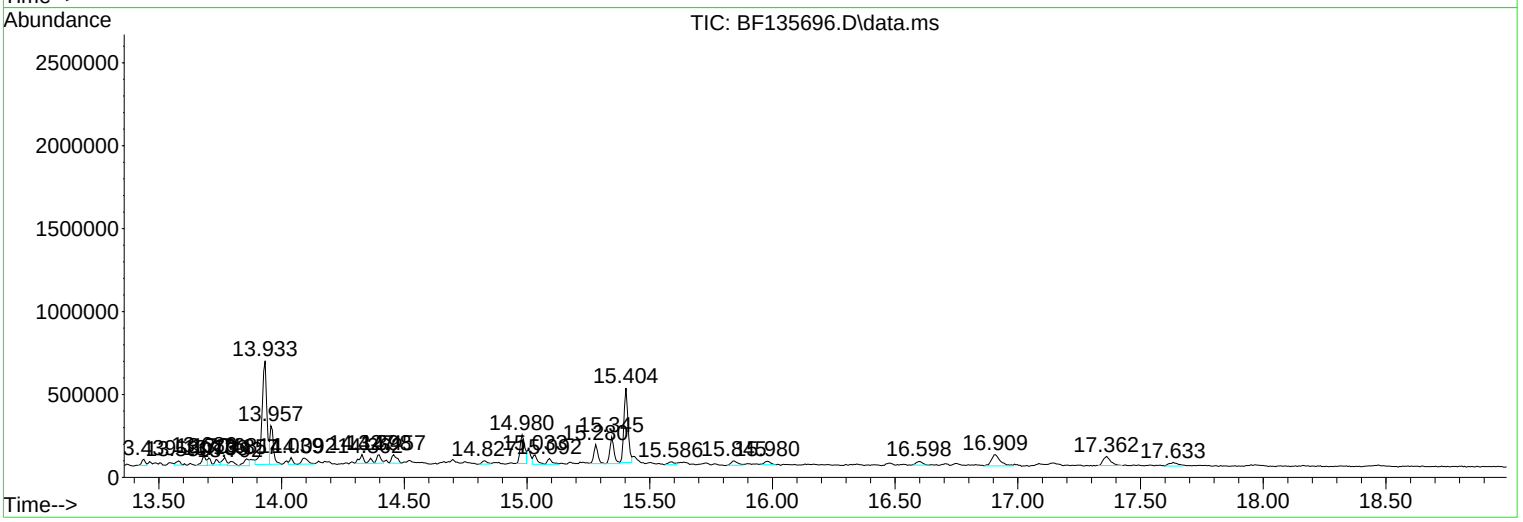
Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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\BF101023\
Data File : BF135696.D
Acq On : 10 Oct 2023 21:09
Operator : CG\JU
Sample : 04753-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

****
Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.775	2.07 ng	65592	1,4-Dichlorobenzene-d4	6.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	90
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	59
3	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	42
4	1-Methoxy-2-propyl acetate	132	C6H12O3	000108-65-6	12
5	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	9

****
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.334	4.18 ng	132197	1,4-Dichlorobenzene-d4	6.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4	Furan, 2,5-dihydro-2,5-dimethyl-	98	C6H10O	059242-27-2	80
5	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	78

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.975	78.42 ng	2481840	1,4-Dichlorobenzene-d4	6.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9

****
Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.763	2.13 ng	67531	1,4-Dichlorobenzene-d4	6.739

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101023\
Data File : BF135696.D
Acq On : 10 Oct 2023 21:09
Operator : CG\JU
Sample : 04753-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	16
3	Heptane	100	C7H16	000142-82-5	9
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
5	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9

****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.216	9.98 ng	416217	Acenaphthene-d10	9.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
3	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	50
4	Metacetamol	151	C8H9NO2	000621-42-1	50
5	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	43

****

Peak Number 6 Anthracene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.774	2.33 ng	100952	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	94
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	93

****

Peak Number 7 Anthracene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	8.21 ng	355581	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	92
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	90

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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	4.70 ng	203757	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	35
3	Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	18
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	18
5	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	18

****
Peak Number 9 Phenanthrene, 2,5-dimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.327	2.01 ng	87214	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	97
2	di-p-Tolylacetylene	206	C16H14	002789-88-0	96
3	9,10-Dimethylanthracene	206	C16H14	000781-43-1	93
4	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	93
5	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	93

****
Peak Number 10 unknown12.368 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.368	2.45 ng	105986	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 4,5,9,10-tetrahydro-	206	C16H14	000781-17-9	38
2	5-Bromo-2-(methylthio)pyrimidine	204	C5H5BrN2S	014001-67-3	38
3	3-Acetyl-2,5-dimethylbenzo(b)thi...	204	C12H12OS	006179-04-0	35
4	Acephenanthrylene, 4,5-dihydro-	204	C16H12	006232-48-0	35
5	Naphthalene, 1-phenyl-	204	C16H12	000605-02-7	35

****
Peak Number 11 Pyrene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.

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Data File : BF135696.D
Acq On : 10 Oct 2023 21:09
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Sample : 04753-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

12.951	2.09 ng	90023	Chrysene-d12	13.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	81
4	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	81
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	80

****

Peak Number 12 11H-Benzo[a]fluorene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.057	2.31 ng	99486	Chrysene-d12	13.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	94
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
5	6H-Thiazolo[5,4-e]indole, 2,7,8-...	216	C12H12N2S	1000338-32-0	64

****

Peak Number 13 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.280	4.93 ng	130361	Perylene-d12	15.403

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
4	Perylene	252	C20H12	000198-55-0	95
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94

Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101023\
Data File : BF135696.D
Acq On : 10 Oct 2023 21:09
Operator : CG\JU
Sample : 04753-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
1,3-Dioxolane, ...	2.775	2.1	ng	65592	1	6.739	632960	20.0
3-Penten-2-one,...	4.334	4.2	ng	132197	1	6.739	632960	20.0
2-Pentanone, 4-...	4.975	78.4	ng	2481840	1	6.739	632960	20.0
2-Pentanone, 4-...	5.763	2.1	ng	67531	1	6.739	632960	20.0
2,4,7,9-Tetrame...	9.216	10.0	ng	416217	3	9.774	834086	20.0
Anthracene, 2-m...	11.774	2.3	ng	100952	4	11.269	866491	20.0
Anthracene, 1-m...	11.804	8.2	ng	355581	4	11.269	866491	20.0
4H-Cyclopenta[d...	11.886	4.7	ng	203757	4	11.269	866491	20.0
Phenanthrene, 2...	12.327	2.0	ng	87214	4	11.269	866491	20.0
unknown12.368	12.368	2.5	ng	105986	4	11.269	866491	20.0
Pyrene, 1-methyl-	12.951	2.1	ng	90023	5	13.933	862571	20.0
11H-Benzo[a]flu...	13.057	2.3	ng	99486	5	13.933	862571	20.0
Benzo[e]pyrene	15.280	4.9	ng	130361	6	15.403	529353	20.0