LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061523\
Data File : BF133781.D
Acq On : 15 Jun 2023 18:28
Operator : CG\JU
Sample : 03221-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-4194

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-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133781.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	17	21	29	rVB	19986	26861	1.10%	0.129%
2	5.045	498	503	515	rVB	85057	112055	4.58%	0.538%
3	5.445	567	571	575	rBV	1990924	2031782	82.97%	9.754%
4	6.463	738	744	754	rBV	1928338	2044352	83.49%	9.814%
5	6.828	803	806	810	rBV	651885	551933	22.54%	2.650%
6	7.392	898	902	905	rBV	1500881	1270144	51.87%	6.097%
7	8.110	1021	1024	1027	rBV	750535	682047	27.85%	3.274%
8	9.192	1204	1208	1211	rBV	2540249	2341970	95.64%	11.243%
9	9.727	1296	1299	1303	rBV	45510	36067	1.47%	0.173%
10	9.869	1319	1323	1326	rBV	846808	677808	27.68%	3.254%
11	9.898	1326	1328	1332	rVB	32694	26917	1.10%	0.129%
12	10.580	1440	1444	1452	rVB	172347	141610	5.78%	0.680%
13	10.657	1453	1457	1466	rVV	1701526	1467248	59.92%	7.044%
14	10.786	1474	1479	1485	rVB3	21162	26509	1.08%	0.127%
15	11.357	1572	1576	1578	rBV	875557	710157	29.00%	3.409%
16	11.380	1578	1580	1583	rVV	205156	162977	6.66%	0.782%
17	11.433	1587	1589	1592	rVB	54896	45408	1.85%	0.218%
18	11.586	1609	1615	1622	rBV	26060	41202	1.68%	0.198%
19	11.857	1656	1661	1663	rBV	53210	54260	2.22%	0.260%
20	11.880	1663	1665	1671	rVB2	266281	260609	10.64%	1.251%
21	11.969	1677	1680	1683	rBV	78209	83478	3.41%	0.401%
22	12.180	1714	1716	1720	rVB	49431	42279	1.73%	0.203%
23	12.410	1752	1755	1758	rBV	48244	50392	2.06%	0.242%
24	12.445	1758	1761	1763	rVV3	33275	34296	1.40%	0.165%
25	12.492	1767	1769	1774	rVB2	53008	57368	2.34%	0.275%
26	12.568	1779	1782	1786	rBV	486130	452382	18.47%	2.172%
27	12.668	1796	1799	1803	rBV2	115137	113622	4.64%	0.545%
28	12.798	1813	1821	1827	rVV	469005	533340	21.78%	2.560%
29	12.851	1827	1830	1834	rVB4	30092	41375	1.69%	0.199%
30	12.945	1842	1846	1850	rVB	2578686	2448754	100.00%	11.756%
31	13.016	1853	1858	1862	rBV4	54040	84163	3.44%	0.404%
32	13.127	1875	1877	1880	rVB2	98735	91337	3.73%	0.438%
33	13.174	1880	1885	1886	rBV2	33914	38733	1.58%	0.186%
34	13.198	1886	1889	1891	rVB	51837	50174	2.05%	0.241%
35	13.233	1891	1895	1898	rBV2	65642	69908	2.85%	0.336%
36	13.327	1907	1911	1913	rBV2	62397	64369	2.63%	0.309%

LSC Area Percent Report

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Acq On : 15 Jun 2023 18:28
Operator : CG\JU
Sample : 03221-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-4194

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-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.357	1913	1916	1919	rVB	43109	40524	1.65%	0.195%
38	13.521	1939	1944	1948	rBV8	27222	57195	2.34%	0.275%
39	13.639	1961	1964	1968	rVB	61969	61738	2.52%	0.296%
40	13.751	1978	1983	1986	rBV3	56402	90669	3.70%	0.435%
41	13.804	1989	1992	1996	rVV2	54406	76561	3.13%	0.368%
42	13.845	1996	1999	2010	rVB2	137990	176933	7.23%	0.849%
43	14.004	2018	2026	2028	rBV2	671376	950523	38.82%	4.563%
44	14.027	2028	2030	2036	rVB	305295	267811	10.94%	1.286%
45	14.104	2041	2043	2045	rBV2	61743	48358	1.97%	0.232%
46	14.421	2095	2097	2100	rBV2	45062	44271	1.81%	0.213%
47	14.627	2129	2132	2136	rBV	149215	179186	7.32%	0.860%
48	14.727	2146	2149	2151	rBV3	49004	52147	2.13%	0.250%
49	14.921	2180	2182	2185	rVB2	45030	32676	1.33%	0.157%
50	15.039	2198	2202	2205	rBV	287126	392368	16.02%	1.884%
51	15.115	2212	2215	2217	rVV	65709	62794	2.56%	0.301%
52	15.145	2217	2220	2226	rVB2	86639	94656	3.87%	0.454%
53	15.339	2249	2253	2258	rBV	172758	203777	8.32%	0.978%
54	15.398	2260	2263	2269	rVB	178205	225550	9.21%	1.083%
55	15.462	2270	2274	2278	rBV	366740	477259	19.49%	2.291%
56	15.927	2350	2353	2359	rVB	48703	73453	3.00%	0.353%
57	16.921	2517	2522	2529	rBV2	74714	159255	6.50%	0.765%
58	17.362	2593	2597	2602	rVB	62088	95025	3.88%	0.456%

Sum of corrected areas: 20830615

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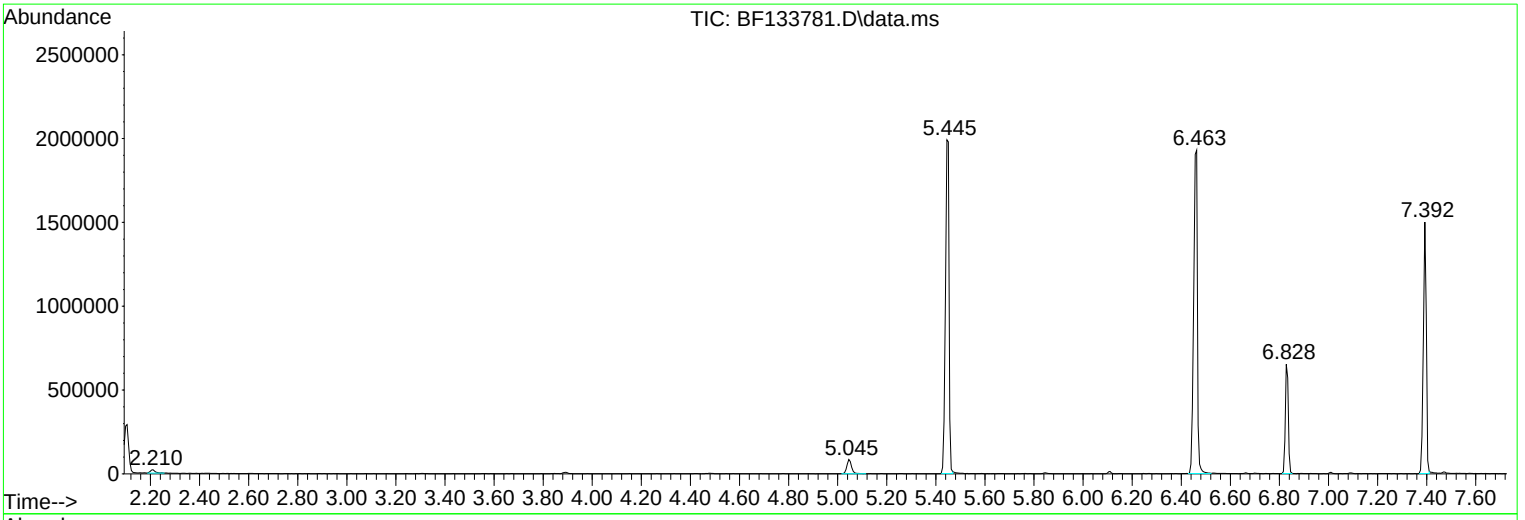
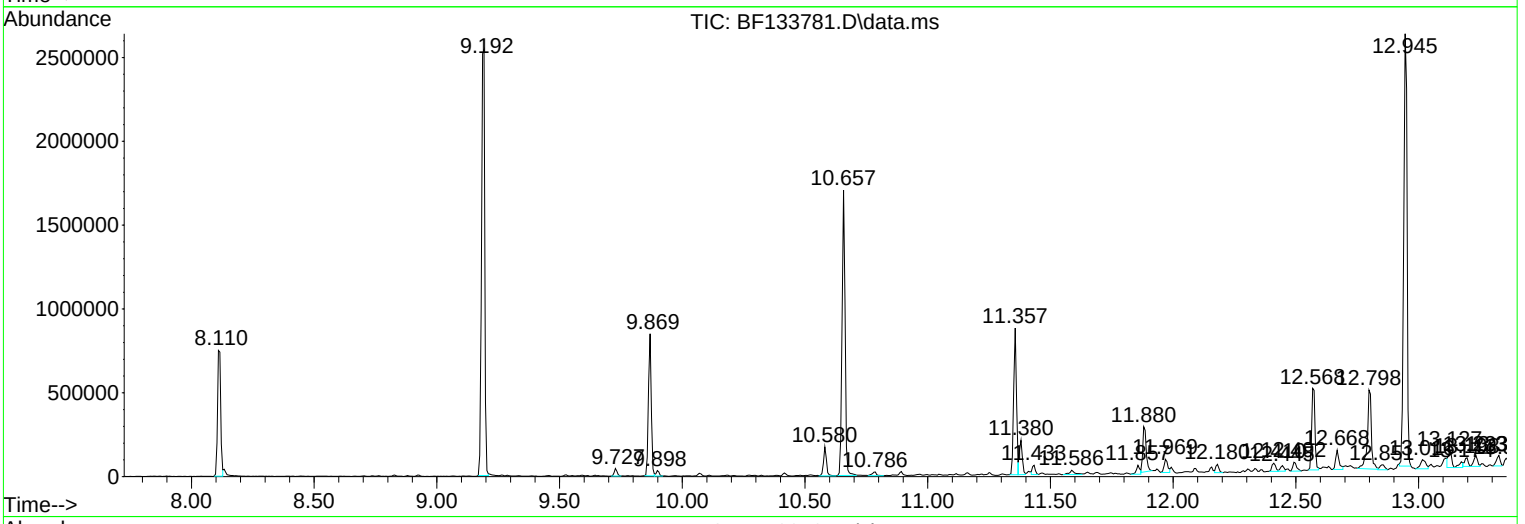
Misc :
ALS Vial : 17 Sample Multiplier: 1

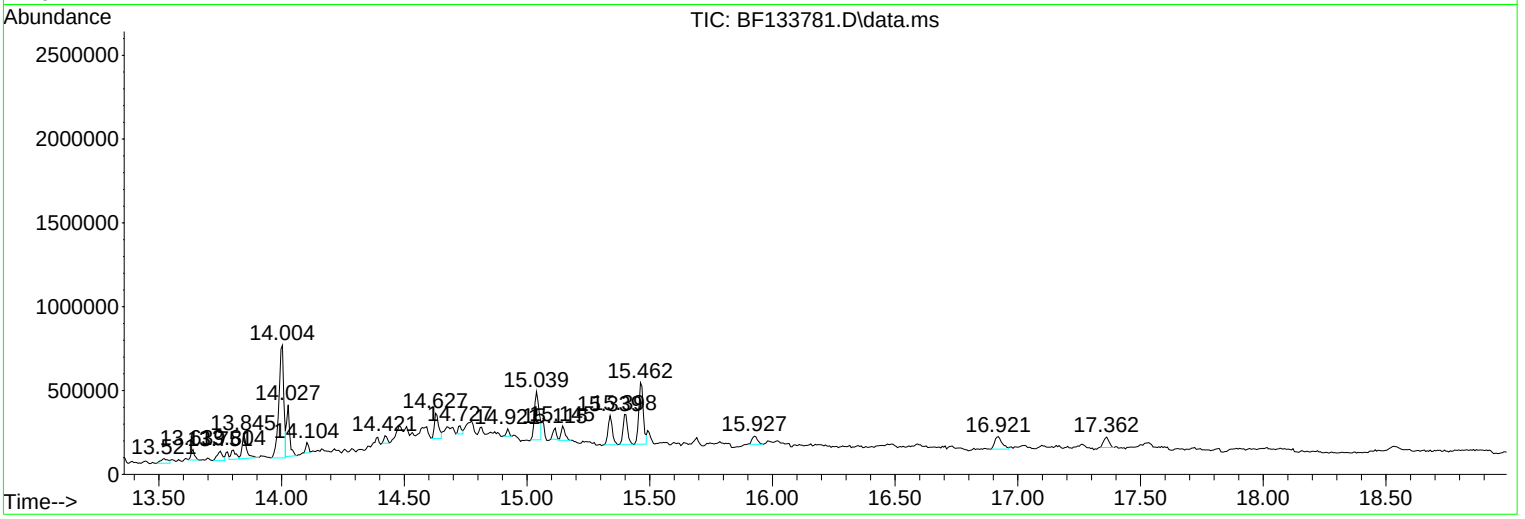
Instrument :
BNA_F
ClientSampleId :
RT-4194

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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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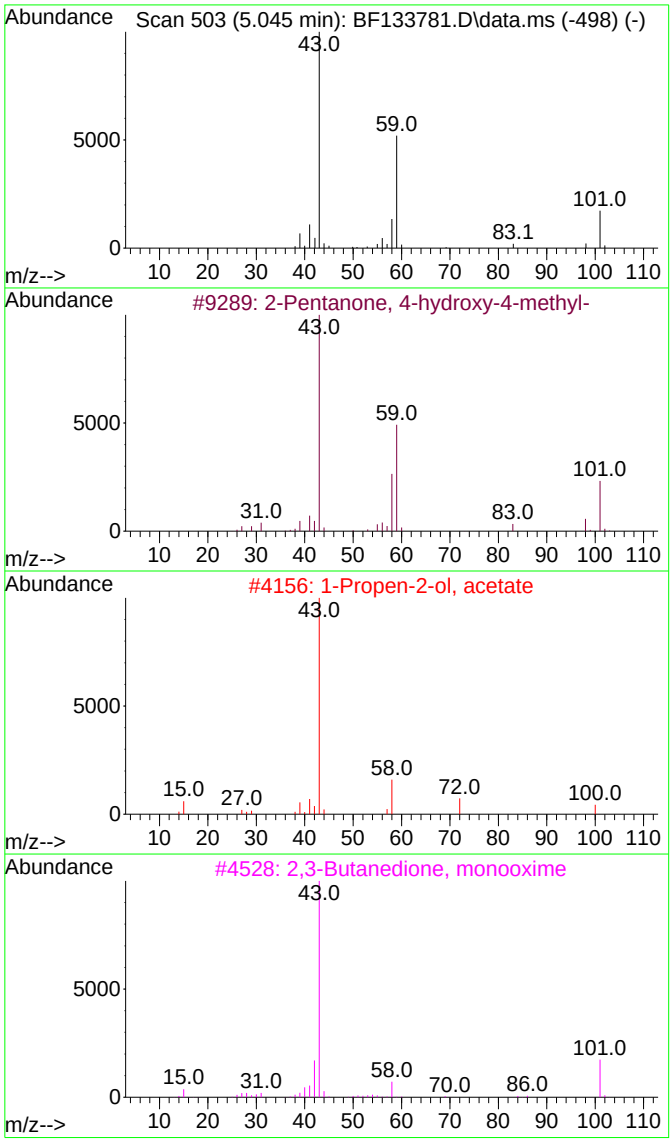
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

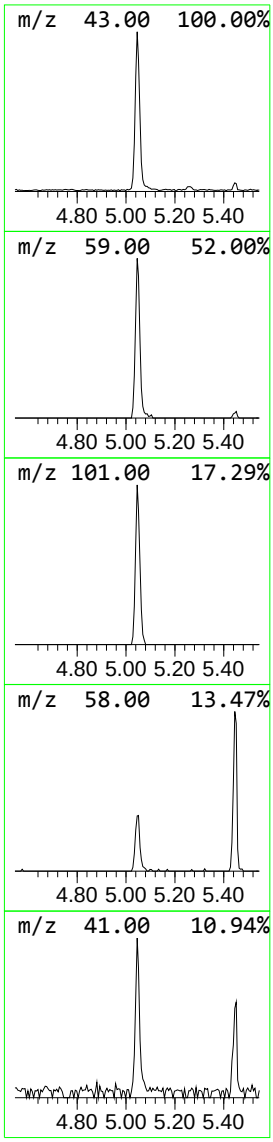
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.045	4.06 ng	112055	1,4-Dichlorobenzene-d4	6.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

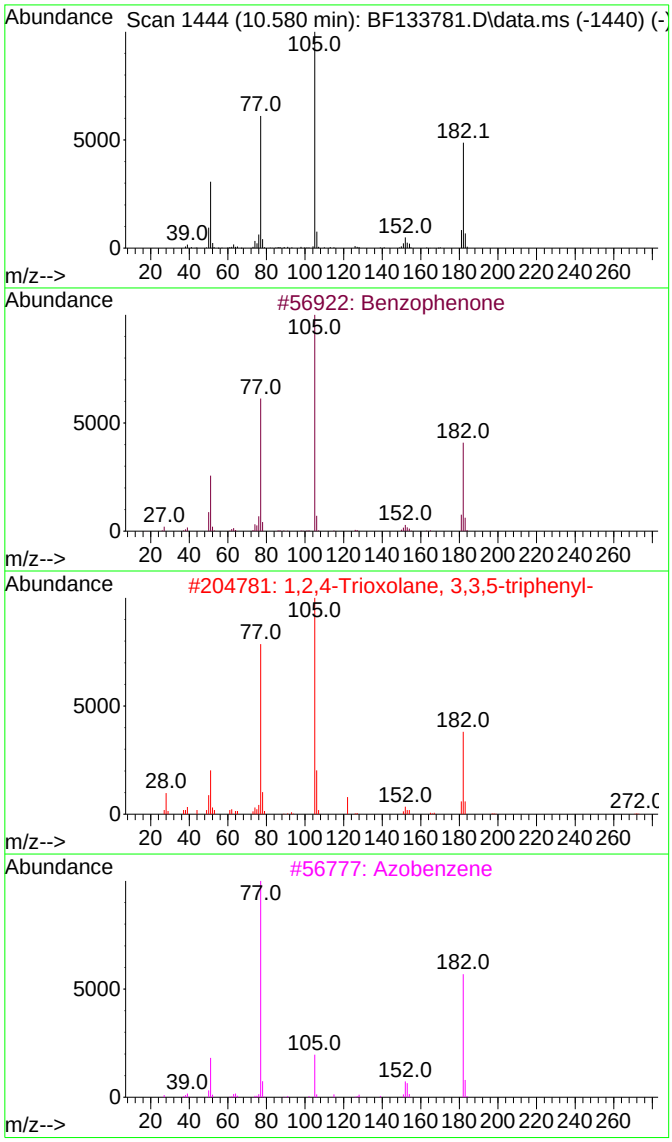
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

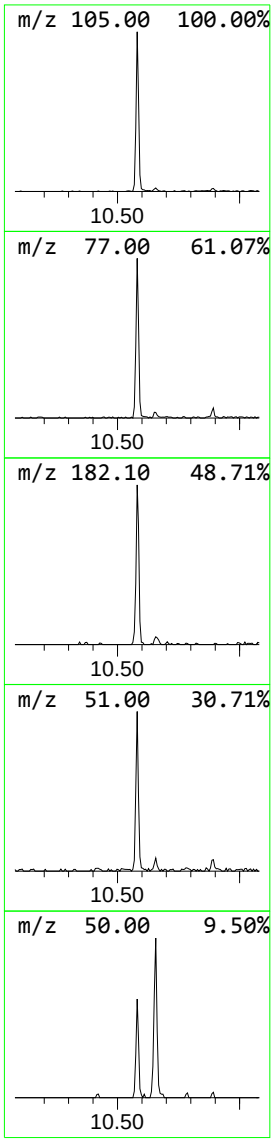
****

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.580	4.18 ng	141610	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	72
3	Azobenzene	182	C12H10N2	000103-33-3	52
4	N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	50
5	N-Methylbenzamide, N-chlorodiflu...	247	C10H8ClF2NO2	1000446-98-2	50





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Sample : 03221-02
Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

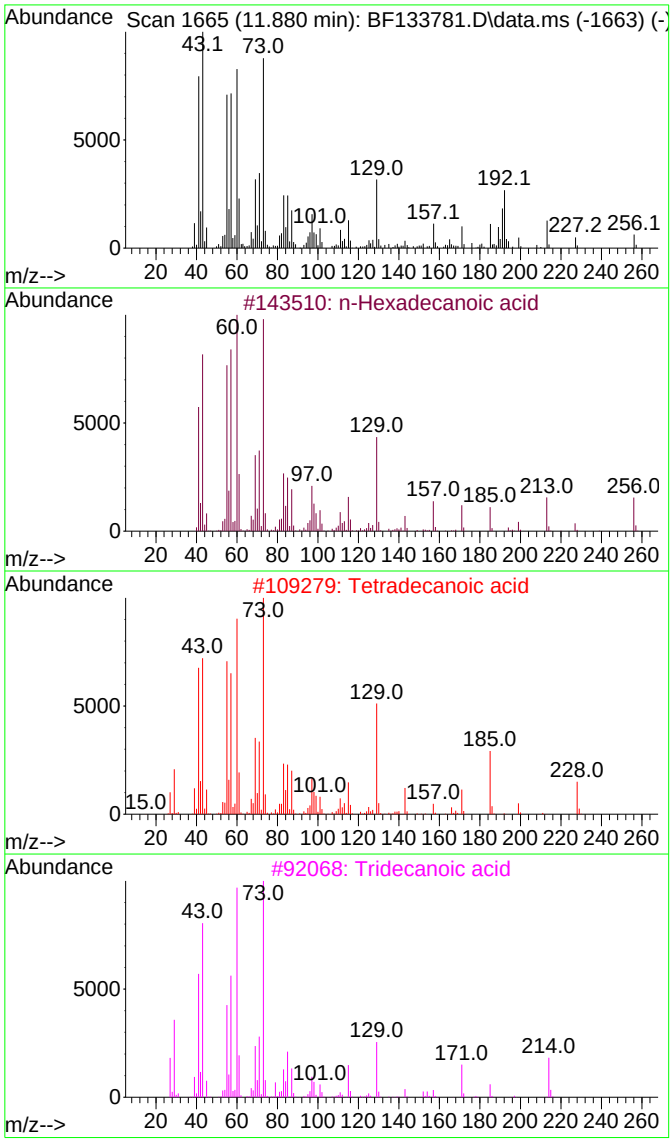
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

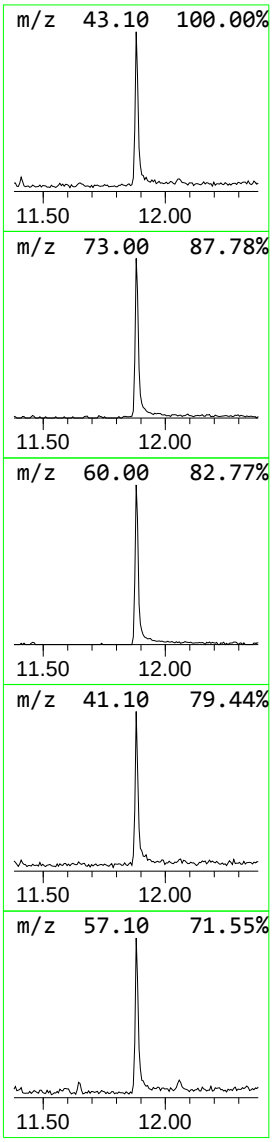
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	7.34 ng	260609	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
3	Tridecanoic acid	214	C13H26O2	000638-53-9	68
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061523\
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

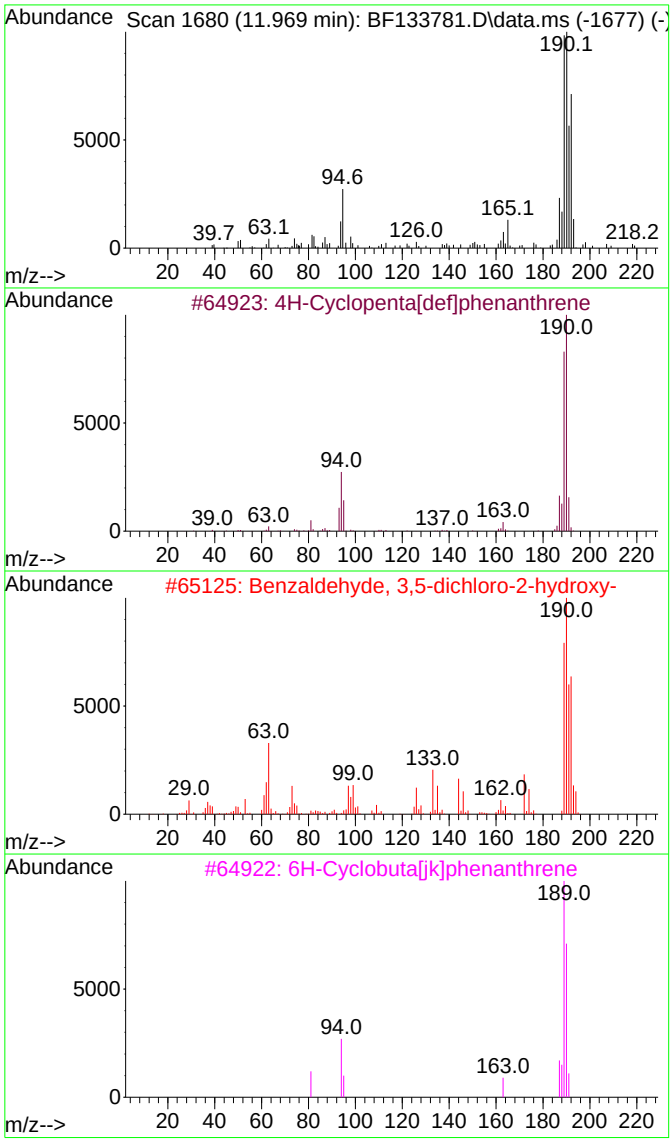
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

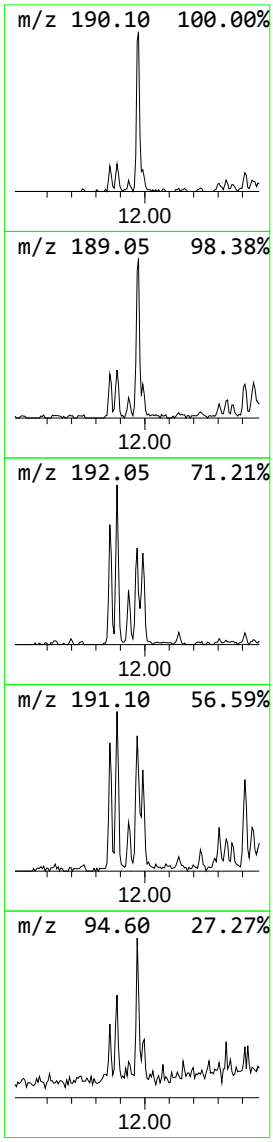
****

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	2.35 ng	83478	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	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	64
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	35
5	Benzene, 1,1'-(2-cyclopropen-1-y...	192	C15H12	022825-21-4	22





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Acq On : 15 Jun 2023 18:28
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Sample : 03221-02
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

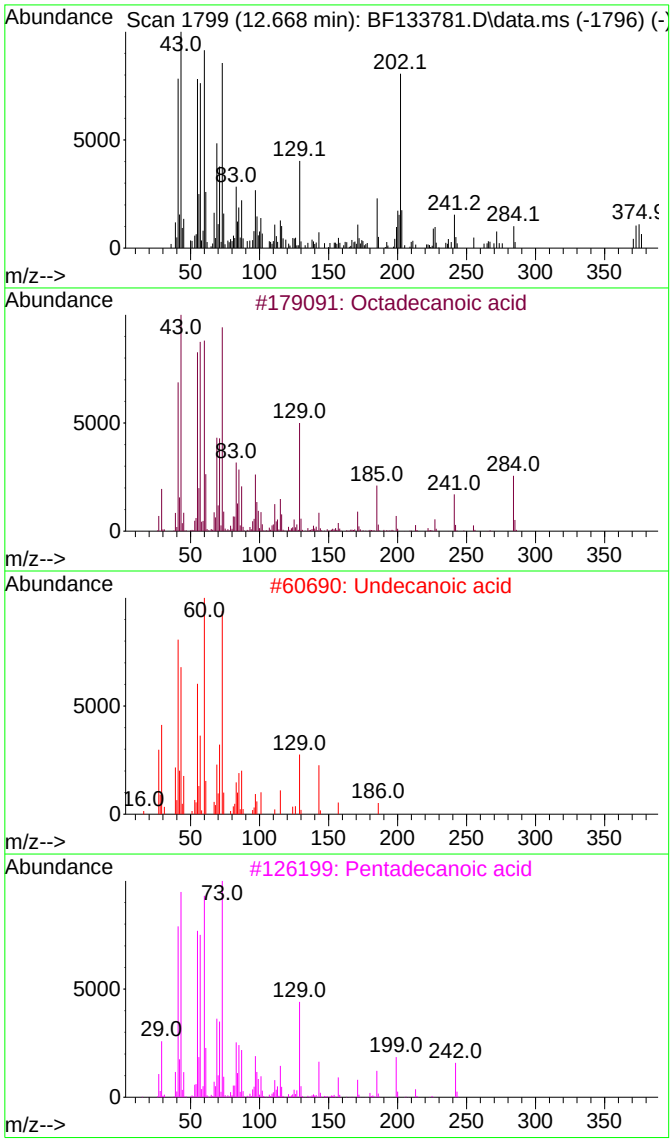
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

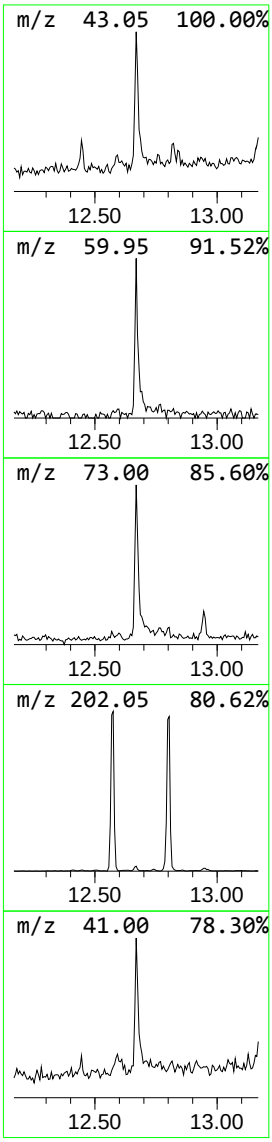
****

Peak Number 5 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.669	3.20 ng	113622	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	Undecanoic acid	186	C11H22O2	000112-37-8	55
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
4	n-Decanoic acid	172	C10H20O2	000334-48-5	46
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	46





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

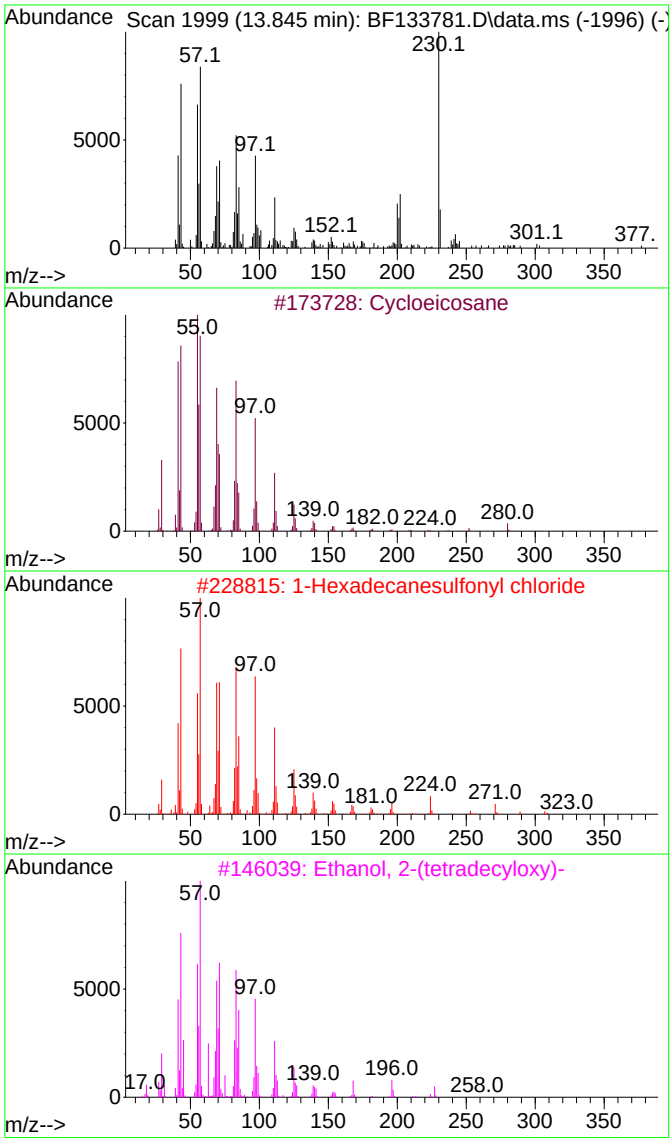
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

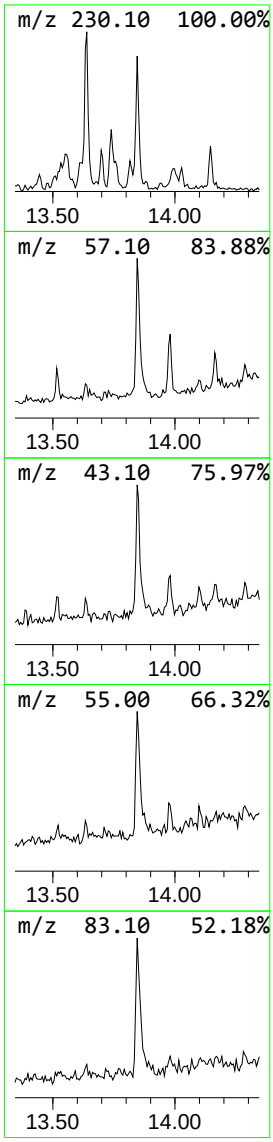
****

Peak Number 6 Cycloeicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	3.72 ng	176933	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	66
2	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	55
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	55
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	50
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	49





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Data File : BF133781.D
Acq On : 15 Jun 2023 18:28
Operator : CG\JU
Sample : 03221-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-4194

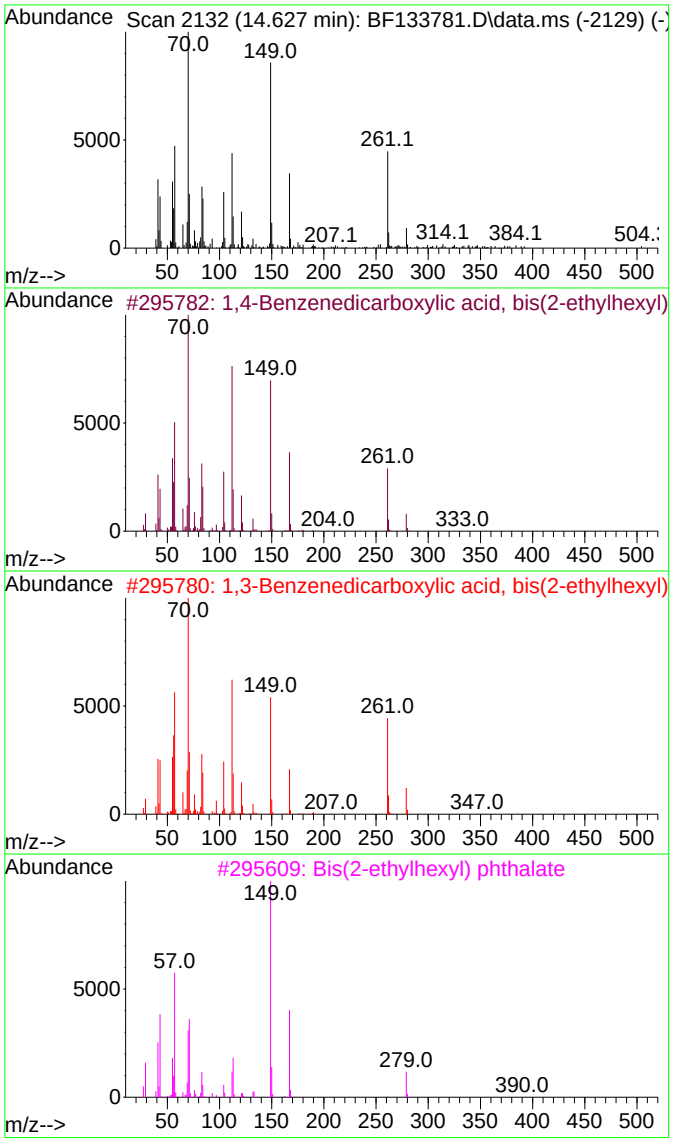
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

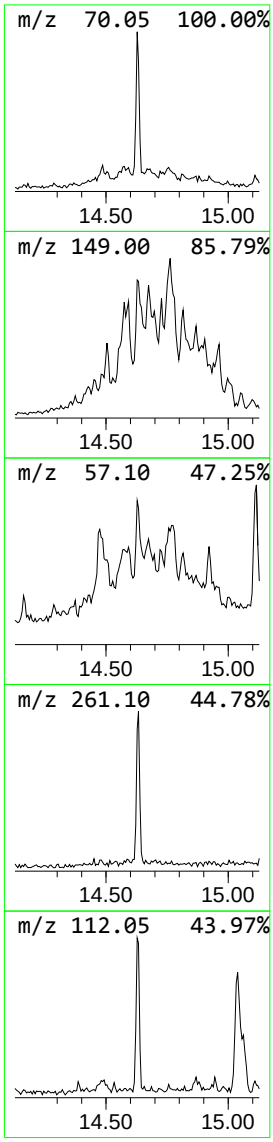
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1,4-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.627	3.77 ng	179186	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	72
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	52
3	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	38
4	Phthalic acid, but-3-yn-2-yl 3,5...	330	C18H12F2O4	1000315-75-6	27
5	Phthalic acid, 6-ethyloct-3-yl 2...	418	C26H42O4	1000315-53-8	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061523\
Data File : BF133781.D
Acq On : 15 Jun 2023 18:28
Operator : CG\JU
Sample : 03221-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-4194

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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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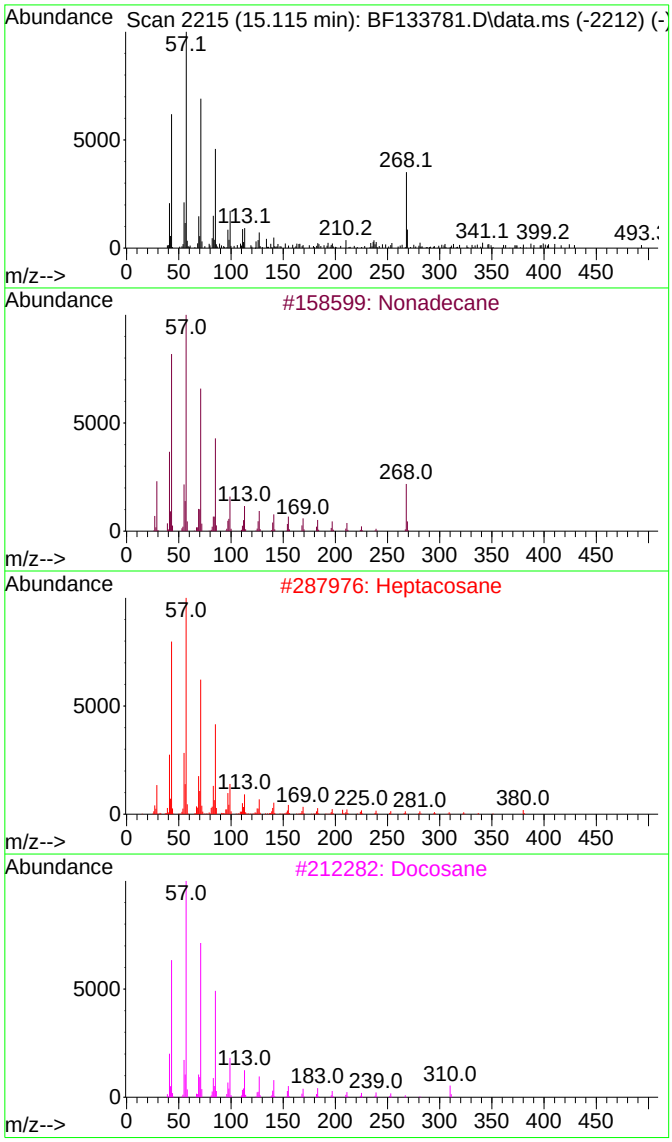
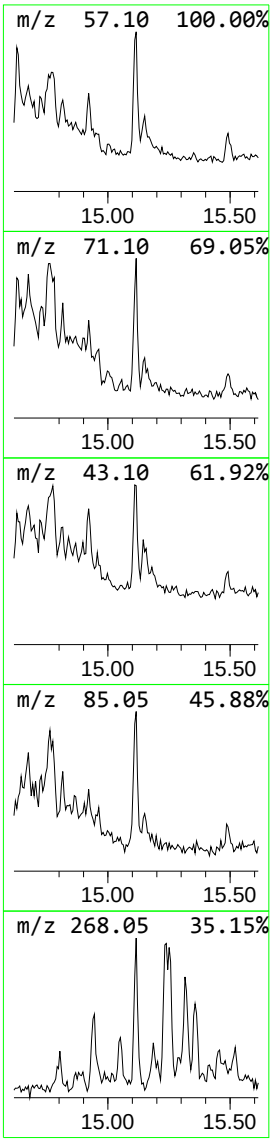
Peak Number 8 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.115	2.63 ng	62794	Perylene-d12	15.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	87
2	Heptacosane	380	C27H56	000593-49-7	83
3	Docosane	310	C22H46	000629-97-0	83
4	Octadecane	254	C18H38	000593-45-3	83
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	58





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Acq On : 15 Jun 2023 18:28
Operator : CG\JU
Sample : 03221-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-4194

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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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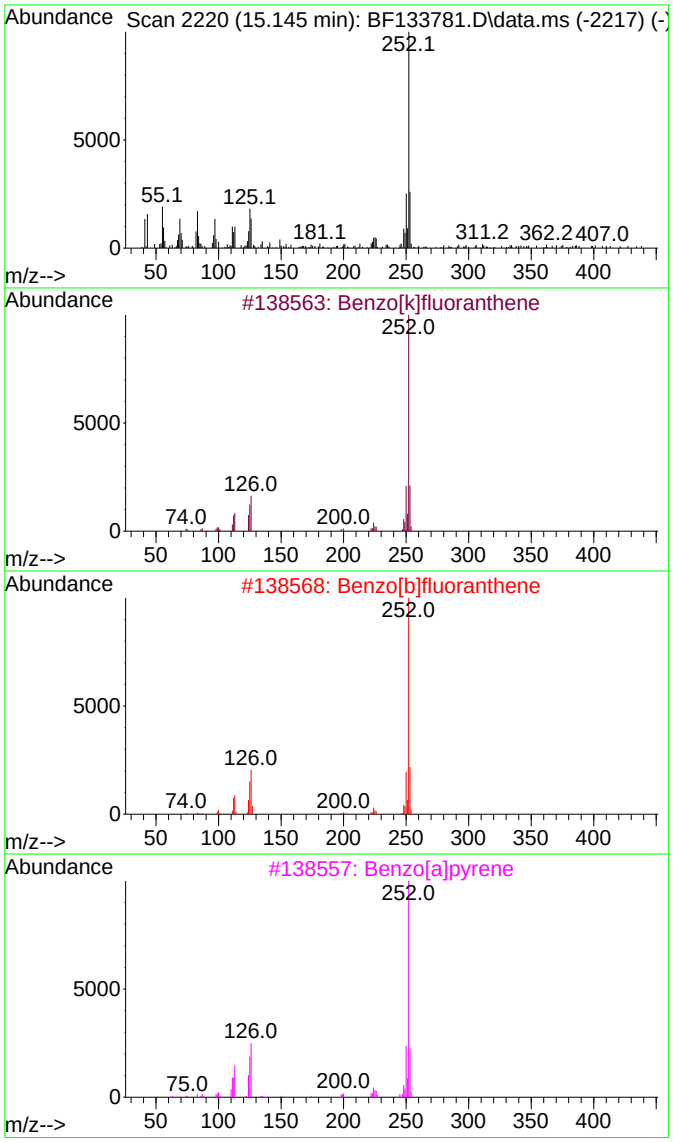
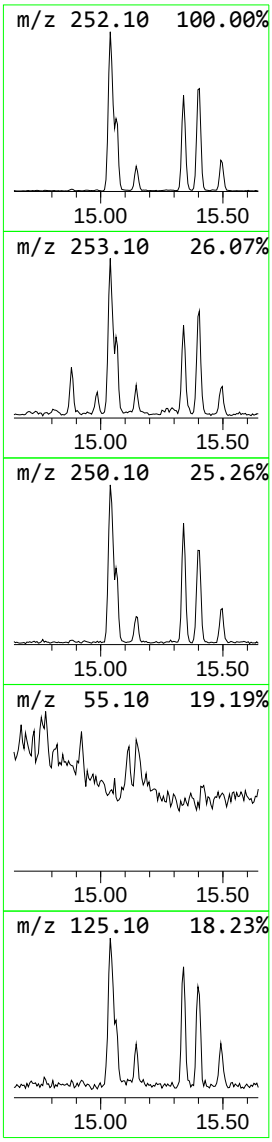
Peak Number 9 Benzo[j]fluoranthene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	3.97 ng	94656	Perylene-d12	15.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
3	Benzo[a]pyrene	252	C20H12	000050-32-8	89
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	89
5	Perylene	252	C20H12	000198-55-0	89





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061523\
Data File : BF133781.D
Acq On : 15 Jun 2023 18:28
Operator : CG\JU
Sample : 03221-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-4194

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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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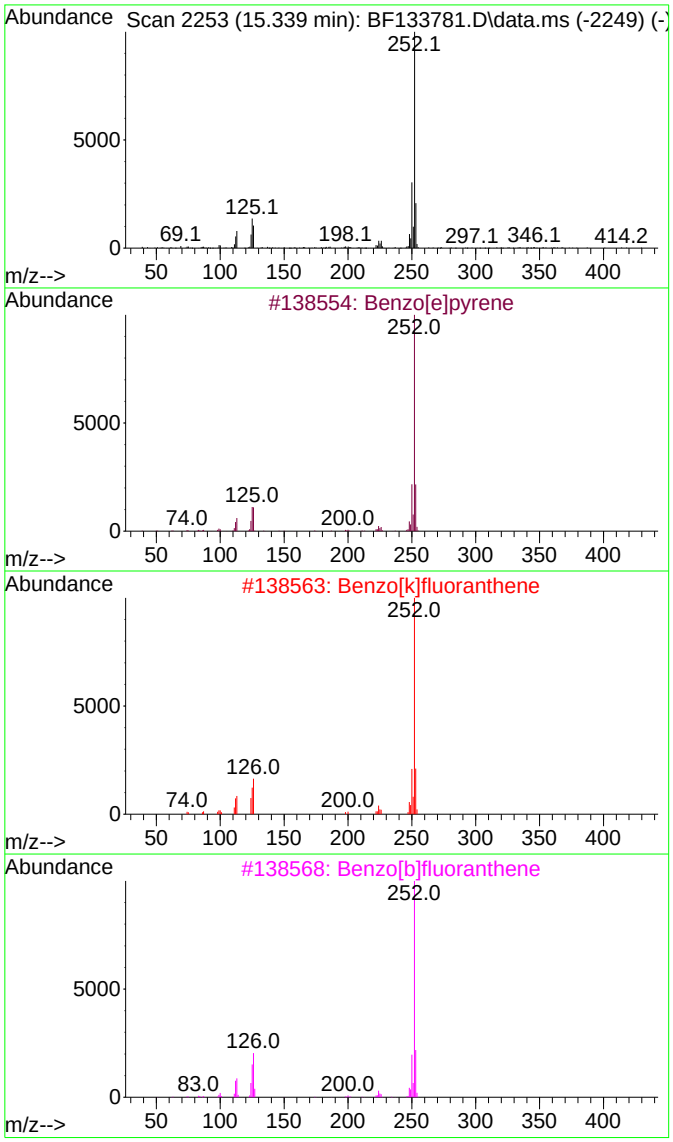
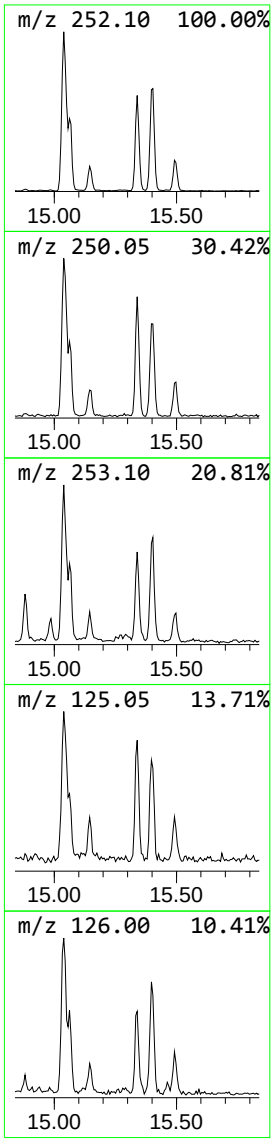
Peak Number 10 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.339	8.54 ng	203777	Perylene-d12	15.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
5	Perylene	252	C20H12	000198-55-0	93





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Data File : BF133781.D
Acq On : 15 Jun 2023 18:28
Operator : CG\JU
Sample : 03221-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-4194

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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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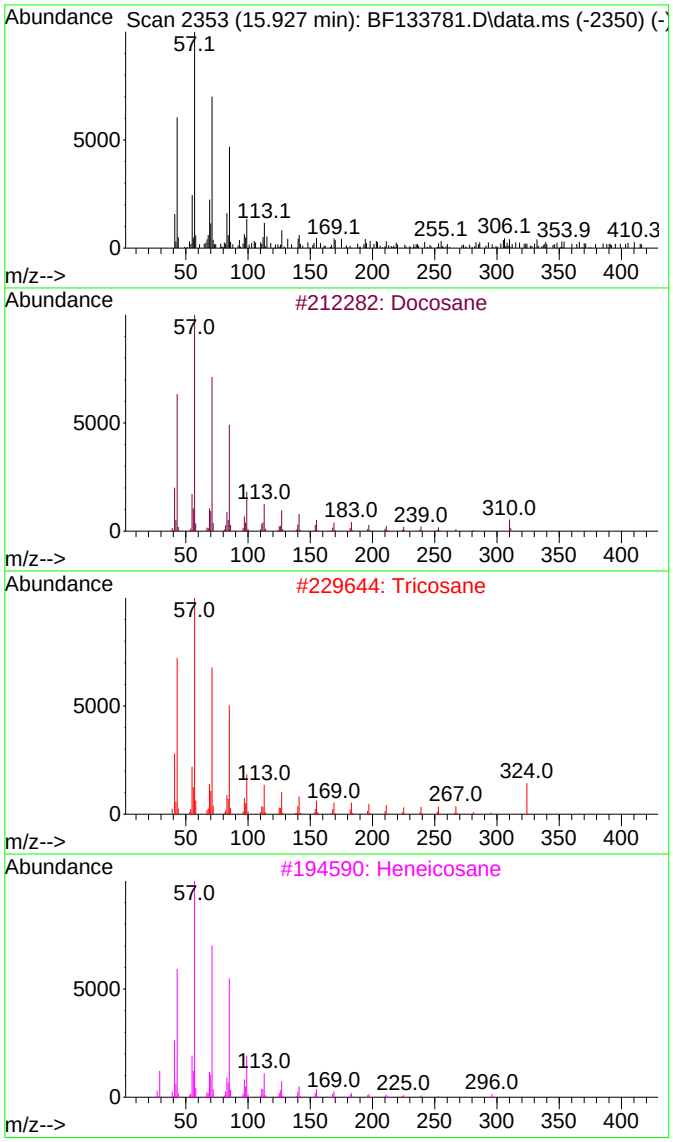
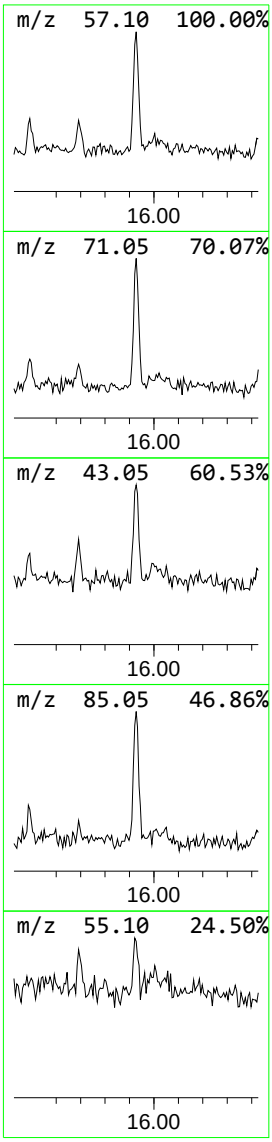
Peak Number 11 Docosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.927	3.08 ng	73453	Perylene-d12	15.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	96
2	Tricosane	324	C23H48	000638-67-5	93
3	Heneicosane	296	C21H44	000629-94-7	93
4	Tetracosane	338	C24H50	000646-31-1	93
5	Hexacosane	366	C26H54	000630-01-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061523\
Data File : BF133781.D
Acq On : 15 Jun 2023 18:28
Operator : CG\JU
Sample : 03221-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-4194

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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
2-Pentanone, 4-...	5.045	4.1	ng	112055	1	6.828	551933	20.0
Benzophenone	10.580	4.2	ng	141610	3	9.869	677808	20.0
n-Hexadecanoic ...	11.880	7.3	ng	260609	4	11.357	710157	20.0
4H-Cyclopenta[d...	11.969	2.4	ng	83478	4	11.357	710157	20.0
Octadecanoic acid	12.669	3.2	ng	113622	4	11.357	710157	20.0
Cycloeicosane	13.845	3.7	ng	176933	5	14.004	950523	20.0
1,4-Benzenedica...	14.627	3.8	ng	179186	5	14.004	950523	20.0
Nonadecane	15.115	2.6	ng	62794	6	15.462	477259	20.0
Benzo[j]fluoran...	15.145	4.0	ng	94656	6	15.462	477259	20.0
Benzo[e]pyrene	15.339	8.5	ng	203777	6	15.462	477259	20.0
Docosane	15.927	3.1	ng	73453	6	15.462	477259	20.0