LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050323\
Data File : BF133218.D
Acq On : 03 May 2023 20:52
Operator : CG\JU
Sample : 02573-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-240

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133218.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.916	477	481	489	rVB	44582	52605	1.42%	0.149%
2	5.340	548	553	556	rBV	3218626	3035424	82.10%	8.616%
3	6.369	723	728	730	rBV	3132722	3200998	86.57%	9.086%
4	6.728	785	789	792	rBV	1515982	1099000	29.72%	3.120%
5	7.293	880	885	888	rBV	2661423	2205496	59.65%	6.260%
6	8.010	1004	1007	1010	rBV	1916675	1491274	40.33%	4.233%
7	9.087	1186	1190	1193	rBV	4387659	3697396	100.00%	10.495%
8	9.539	1265	1267	1273	rVB2	38467	44174	1.19%	0.125%
9	9.622	1278	1281	1284	rVV	61875	47474	1.28%	0.135%
10	9.763	1301	1305	1308	rBV	2084098	1640454	44.37%	4.657%
11	9.792	1308	1310	1314	rVB	73920	59504	1.61%	0.169%
12	10.310	1394	1398	1403	rVB2	63587	65930	1.78%	0.187%
13	10.475	1422	1426	1429	rBV	1825164	1455481	39.37%	4.131%
14	10.551	1435	1439	1445	rBV	1163107	1022127	27.64%	2.901%
15	10.675	1456	1460	1468	rVB6	49288	59846	1.62%	0.170%
16	10.781	1475	1478	1483	rBV	219915	185437	5.02%	0.526%
17	10.869	1487	1493	1497	rBV	223513	274607	7.43%	0.779%
18	11.051	1521	1524	1528	rVB	46707	47784	1.29%	0.136%
19	11.163	1541	1543	1547	rVB	131090	110721	2.99%	0.314%
20	11.245	1553	1557	1559	rBV	1841956	1507292	40.77%	4.279%
21	11.269	1559	1561	1564	rVV	1011123	730827	19.77%	2.074%
22	11.316	1566	1569	1573	rVB	111899	104613	2.83%	0.297%
23	11.475	1593	1596	1599	rBV	73546	64615	1.75%	0.183%
24	11.575	1610	1613	1619	rVB	68658	62701	1.70%	0.178%
25	11.657	1624	1627	1630	rVB	39178	45548	1.23%	0.129%
26	11.745	1639	1642	1644	rBV	167967	148381	4.01%	0.421%
27	11.775	1644	1647	1652	rVV	246687	257433	6.96%	0.731%
28	11.816	1652	1654	1657	rVV2	53483	60183	1.63%	0.171%
29	11.857	1657	1661	1663	rVV2	234568	245898	6.65%	0.698%
30	11.880	1663	1665	1670	rVB	128566	106178	2.87%	0.301%
31	12.039	1690	1692	1694	rBV	88503	83106	2.25%	0.236%
32	12.063	1694	1696	1703	rVB2	155295	143098	3.87%	0.406%
33	12.298	1732	1736	1738	rBV	115631	118996	3.22%	0.338%
34	12.327	1738	1741	1743	rVV2	62629	81147	2.19%	0.230%
35	12.351	1743	1745	1747	rVV2	61172	50930	1.38%	0.145%
36	12.375	1747	1749	1754	rVV3	76710	96539	2.61%	0.274%

LSC Area Percent Report

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Data File : BF133218.D
Acq On : 03 May 2023 20:52
Operator : CG\JU
Sample : 02573-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-240

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.457	1759	1763	1766	rVB	1103381	983387	26.60%	2.791%
38	12.563	1776	1781	1783	rBV3	64598	106742	2.89%	0.303%
39	12.604	1786	1788	1793	rVB3	46566	51039	1.38%	0.145%
40	12.680	1796	1801	1804	rBV	994848	960639	25.98%	2.727%
41	12.739	1809	1811	1815	rVB2	58294	70665	1.91%	0.201%
42	12.833	1823	1827	1830	rBV	2701873	2529268	68.41%	7.179%
43	12.904	1834	1839	1842	rBV2	79422	122751	3.32%	0.348%
44	12.992	1850	1854	1855	rBV3	63404	77966	2.11%	0.221%
45	13.010	1855	1857	1860	rVB	137569	114959	3.11%	0.326%
46	13.074	1861	1868	1871	rBV3	128643	157809	4.27%	0.448%
47	13.116	1871	1875	1878	rBV2	122159	136328	3.69%	0.387%
48	13.204	1888	1890	1893	rVB	68634	61775	1.67%	0.175%
49	13.239	1893	1896	1899	rBV	69257	65402	1.77%	0.186%
50	13.416	1923	1926	1928	rBV	65370	50281	1.36%	0.143%
51	13.516	1940	1943	1948	rVB	91766	99211	2.68%	0.282%
52	13.627	1957	1962	1965	rBV2	106835	135108	3.65%	0.384%
53	13.680	1969	1971	1975	rVV2	50342	57295	1.55%	0.163%
54	13.722	1975	1978	1980	rVV2	72953	64544	1.75%	0.183%
55	13.798	1984	1991	1998	rBV6	74222	223020	6.03%	0.633%
56	13.880	1999	2005	2007	rBV2	1228319	1425605	38.56%	4.047%
57	13.904	2007	2009	2012	rVB	418105	316603	8.56%	0.899%
58	14.063	2033	2036	2039	rVB3	61923	68280	1.85%	0.194%
59	14.263	2066	2070	2073	rBV	89667	102285	2.77%	0.290%
60	14.298	2073	2076	2080	rVB2	64039	61678	1.67%	0.175%
61	14.363	2084	2087	2089	rBV3	87392	79628	2.15%	0.226%
62	14.392	2089	2092	2094	rBV	57484	48905	1.32%	0.139%
63	14.663	2136	2138	2145	rVB3	70387	91749	2.48%	0.260%
64	14.733	2146	2150	2155	rBV3	87421	142944	3.87%	0.406%
65	14.798	2159	2161	2172	rVB7	62209	104431	2.82%	0.296%
66	14.892	2173	2177	2180	rBV	372083	526060	14.23%	1.493%
67	14.986	2189	2193	2199	rVB3	96671	164783	4.46%	0.468%
68	15.180	2222	2226	2232	rVB	235472	286786	7.76%	0.814%
69	15.239	2232	2236	2241	rBV	302717	342775	9.27%	0.973%
70	15.298	2241	2246	2250	rVV	907681	1045994	28.29%	2.969%
71	15.327	2250	2251	2260	rVB2	90174	130777	3.54%	0.371%
72	15.633	2301	2303	2310	rVB3	43126	67374	1.82%	0.191%
73	15.757	2320	2324	2328	rBV	74239	102454	2.77%	0.291%
74	16.668	2474	2479	2488	rVB3	98613	210391	5.69%	0.597%
75	17.080	2545	2549	2557	rVB2	71785	138301	3.74%	0.393%

LSC Area Percent Report

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Acq On : 03 May 2023 20:52
Operator : CG\JU
Sample : O2573-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-240

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

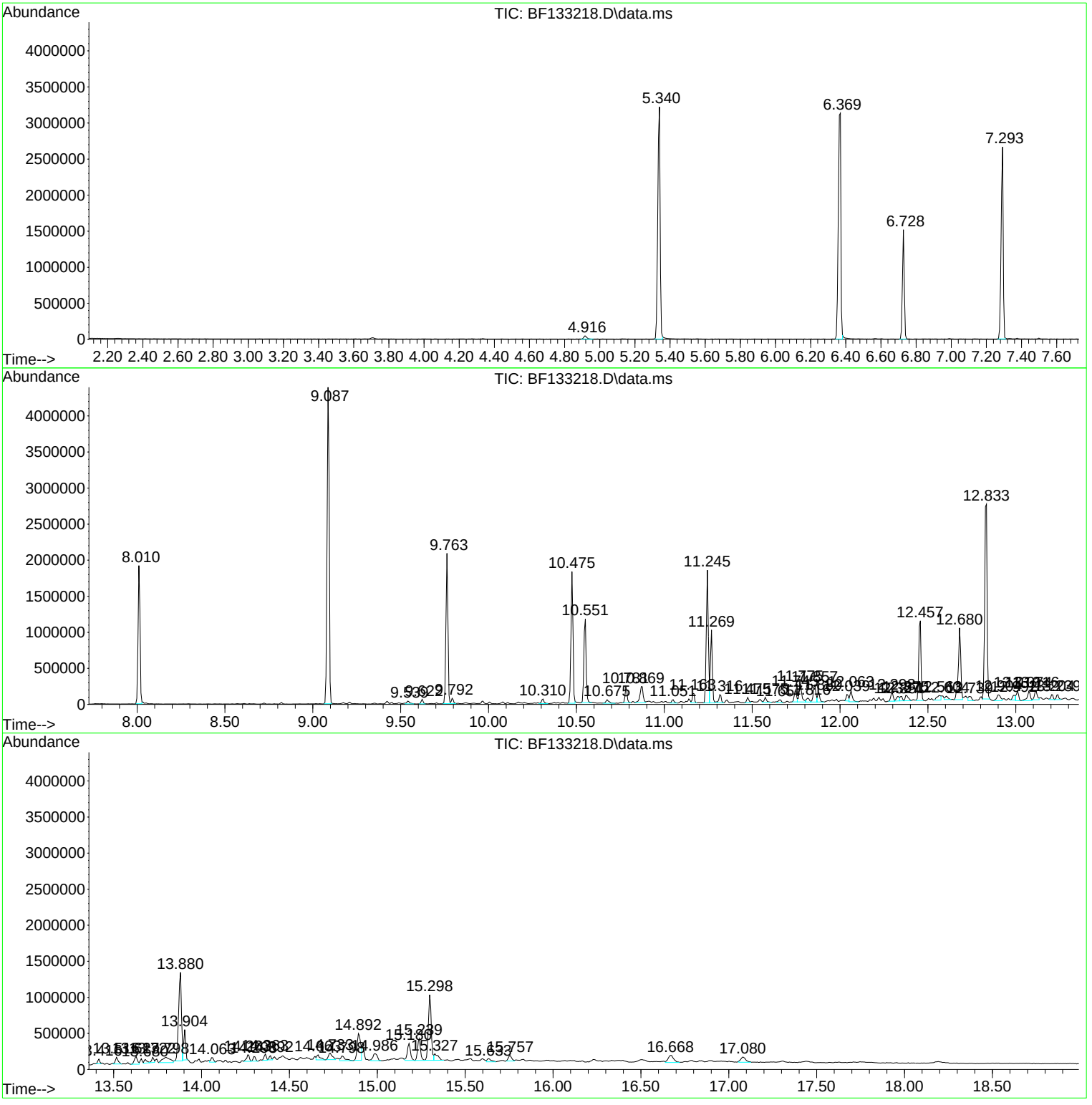
Sum of corrected areas: 35229209

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050323\
Data File : BF133218.D
Acq On : 03 May 2023 20:52
Operator : CG\JU
Sample : 02573-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-240

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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\BF050323\
Data File : BF133218.D
Acq On : 03 May 2023 20:52
Operator : CG\JU
Sample : 02573-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-240

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

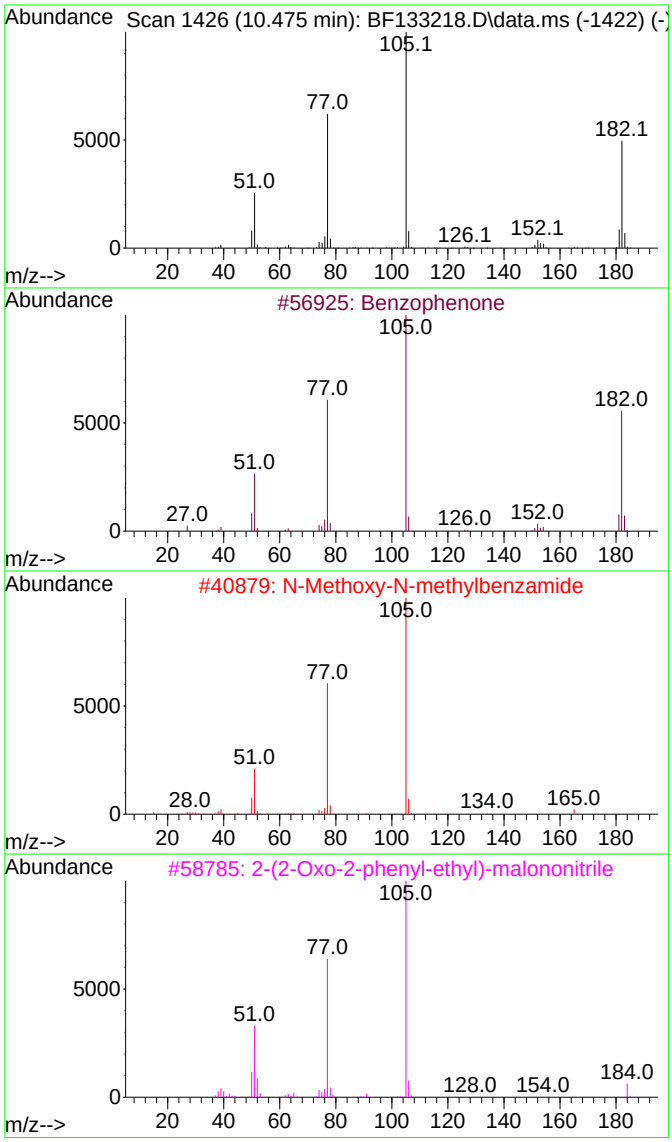
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

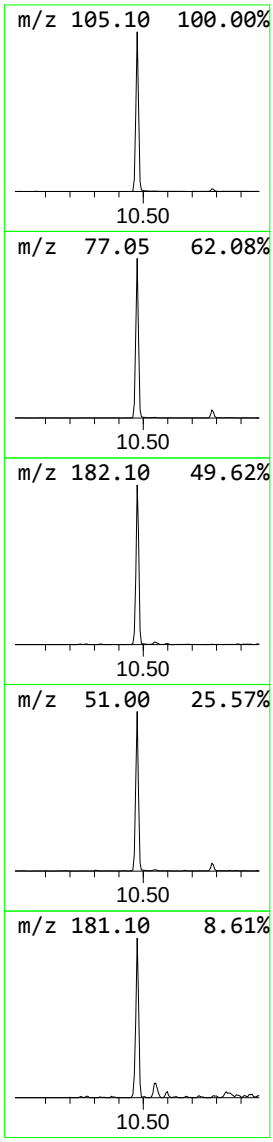
****

Peak Number 1 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	17.74 ng	1455480	Acenaphthene-d10	9.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
3	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
4	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
5	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050323\
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Instrument :
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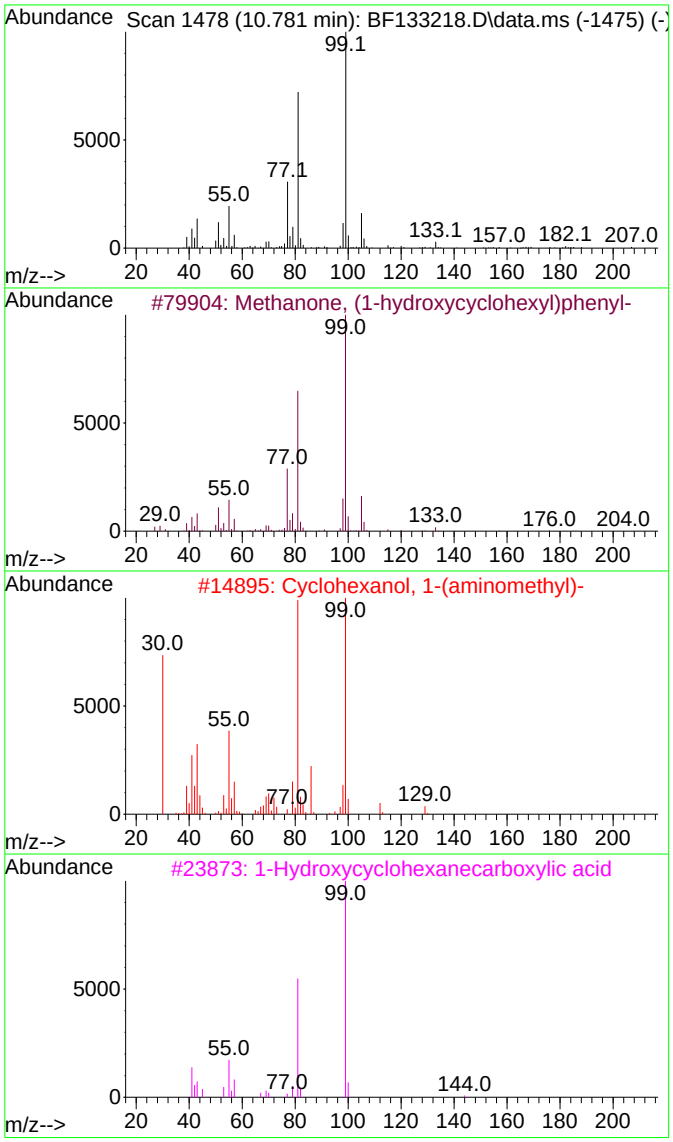
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

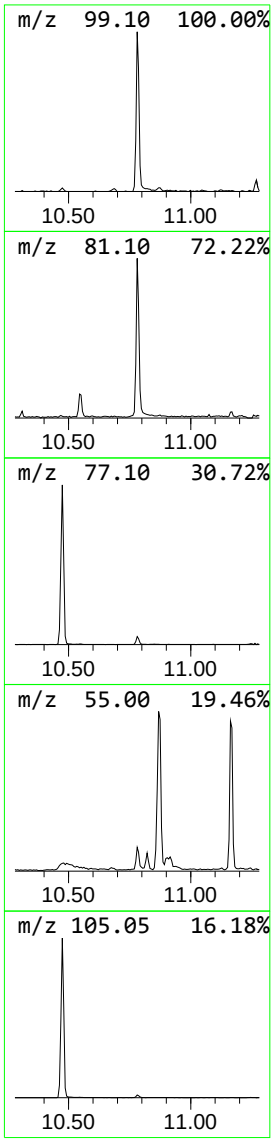
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Methanone, (1-hydroxycycloh... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.781	2.46 ng	185437	Phenanthrene-d10	11.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	91
2	Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	53
3	1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	40
4	Cyclohexanol, 1-ethyl-	128	C8H16O	001940-18-7	40
5	Hexanoic acid, thio-, S-butyl ester	188	C10H20OS	002432-79-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050323\
Data File : BF133218.D
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Operator : CG\JU
Sample : 02573-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-240

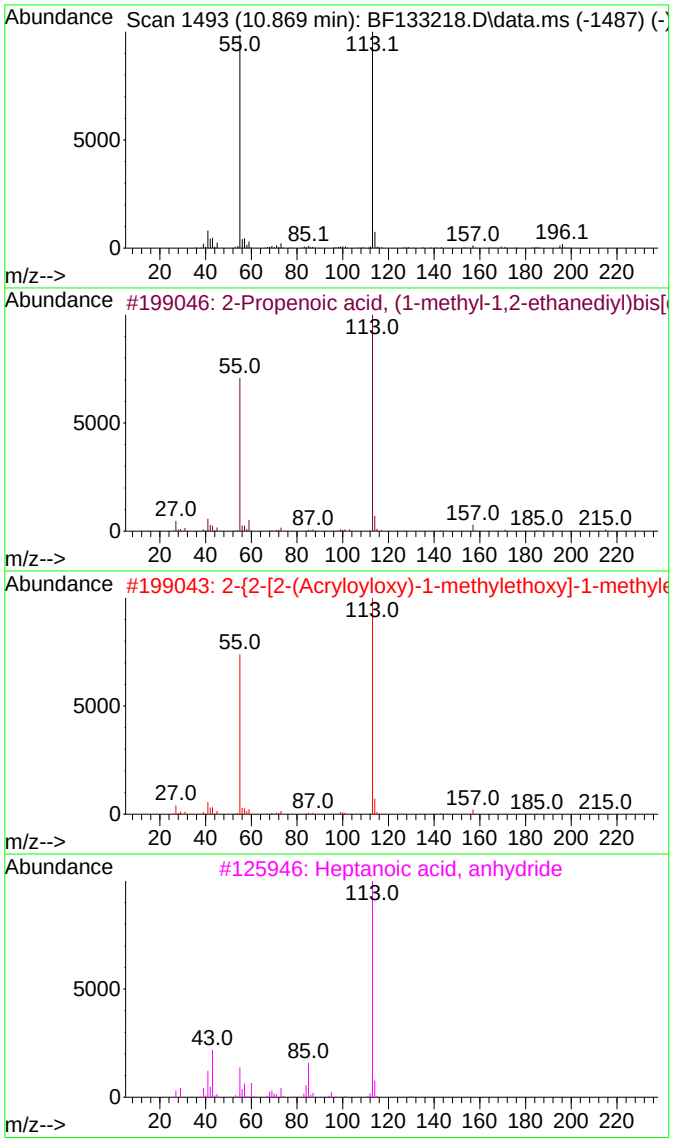
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

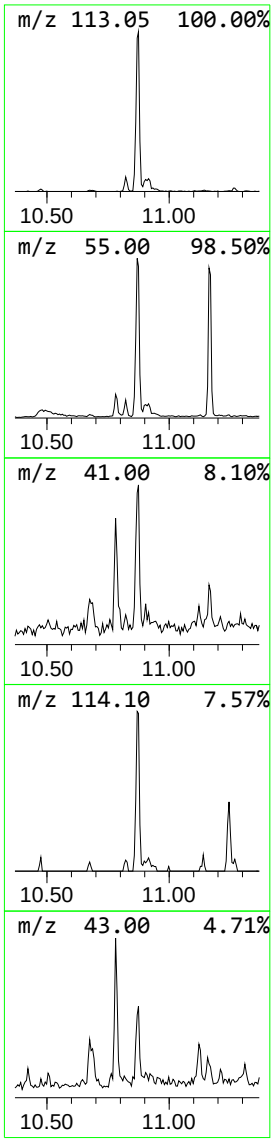
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propenoic acid, (1-methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.869	3.64 ng	274607	Phenanthrene-d10	11.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, (1-methyl-1,2-...	300	C15H24O6	042978-66-5	72
2	2-{2-[2-(Acryloyloxy)-1-methylet...	300	C15H24O6	094120-00-0	72
3	Heptanoic acid, anhydride	242	C14H26O3	000626-27-7	36
4	1-(3-Cyclopentylpropanoyl)pyrrol...	195	C12H21NO	544683-75-2	9
5	(E)1-Allyl-2-methylcyclohexanol	154	C10H18O	1000311-73-7	9





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

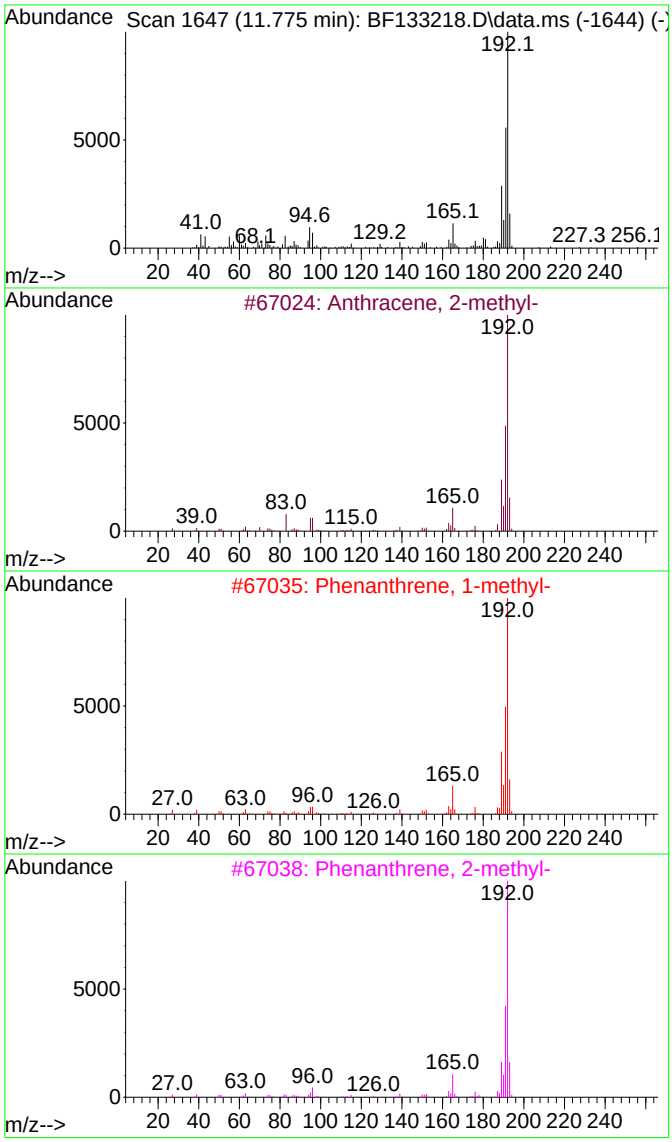
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

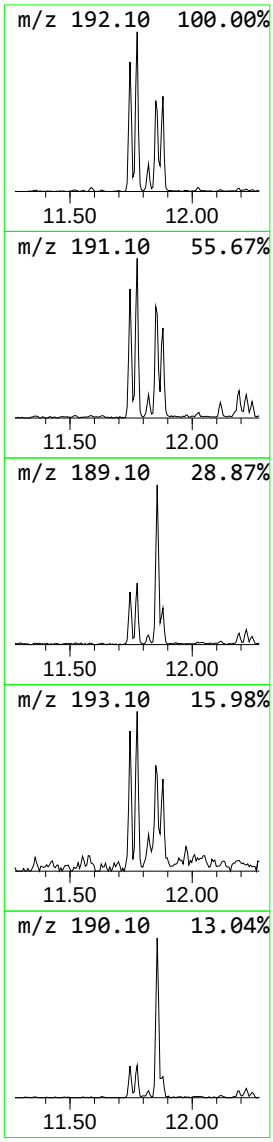
****

Peak Number 4 Anthracene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.775	3.42 ng	257433	Phenanthrene-d10	11.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
4	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	94
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	94





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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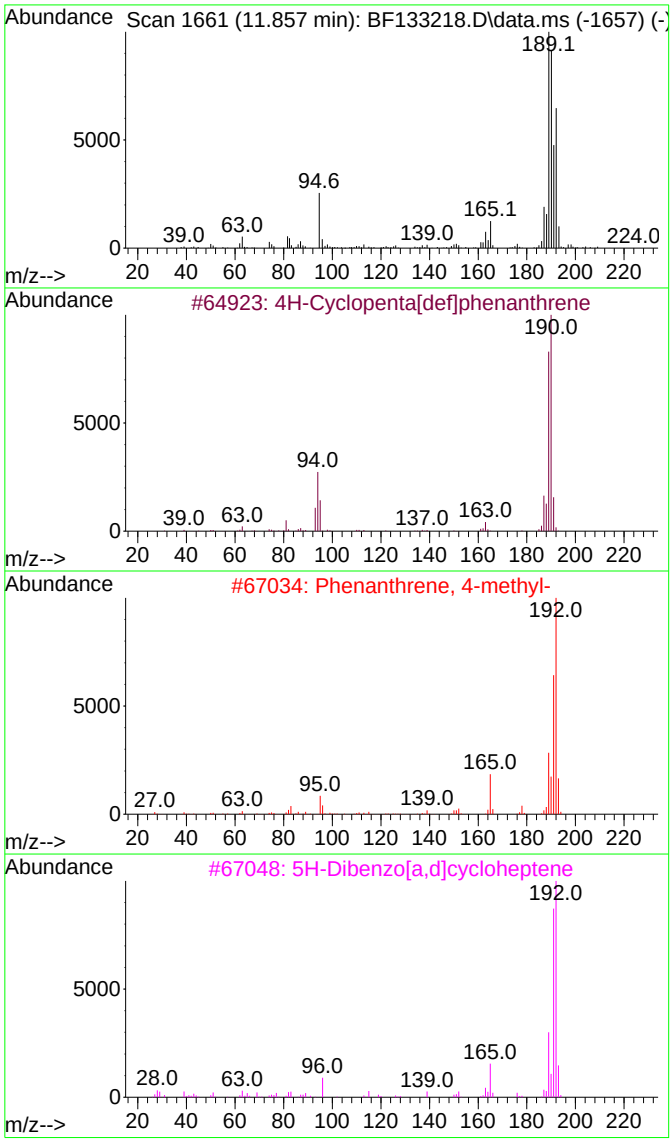
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

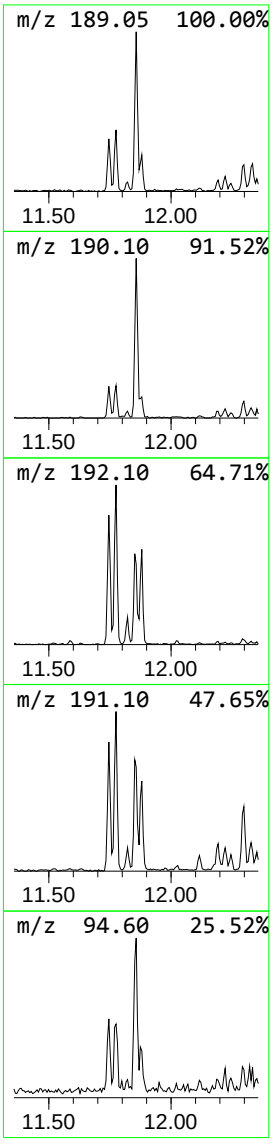
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	3.26 ng	245898	Phenanthrene-d10	11.245

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	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	25
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	25
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	25





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Data File : BF133218.D
Acq On : 03 May 2023 20:52
Operator : CG\JU
Sample : 02573-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-240

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

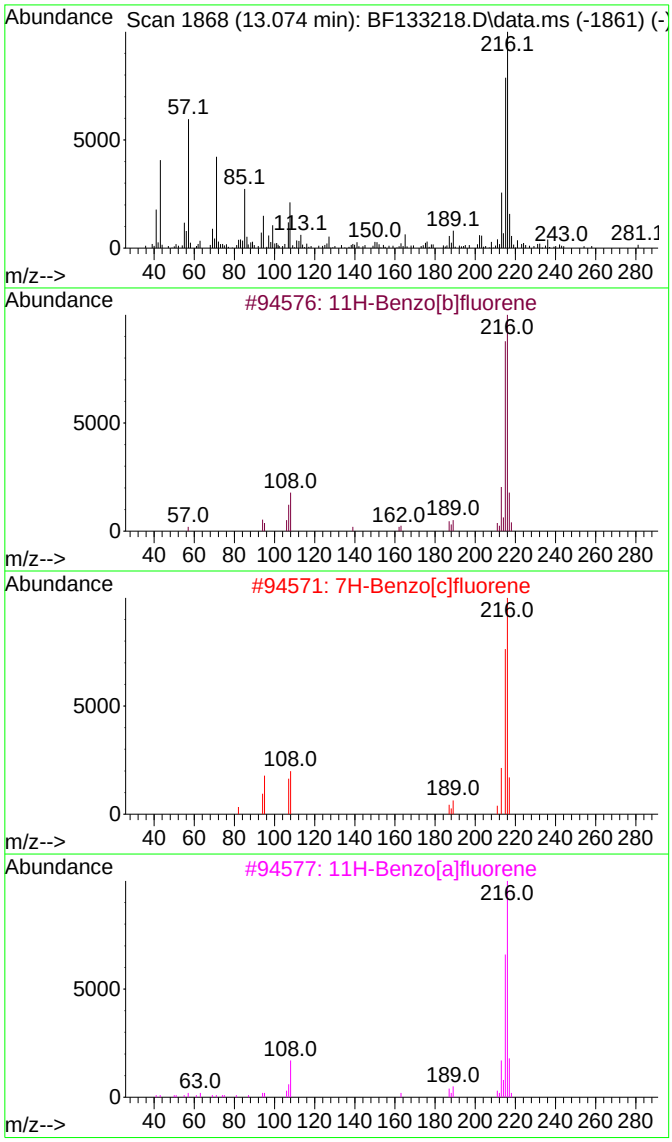
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

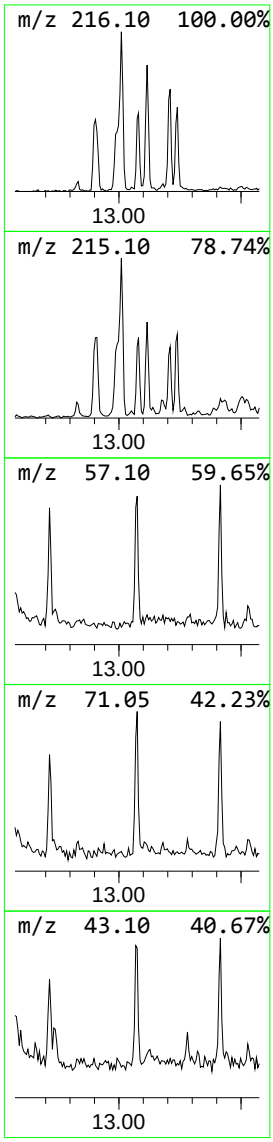
****

Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.075	2.21 ng	157809	Chrysene-d12	13.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
2	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	93
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	92
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	92
5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050323\
Data File : BF133218.D
Acq On : 03 May 2023 20:52
Operator : CG\JU
Sample : 02573-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-240

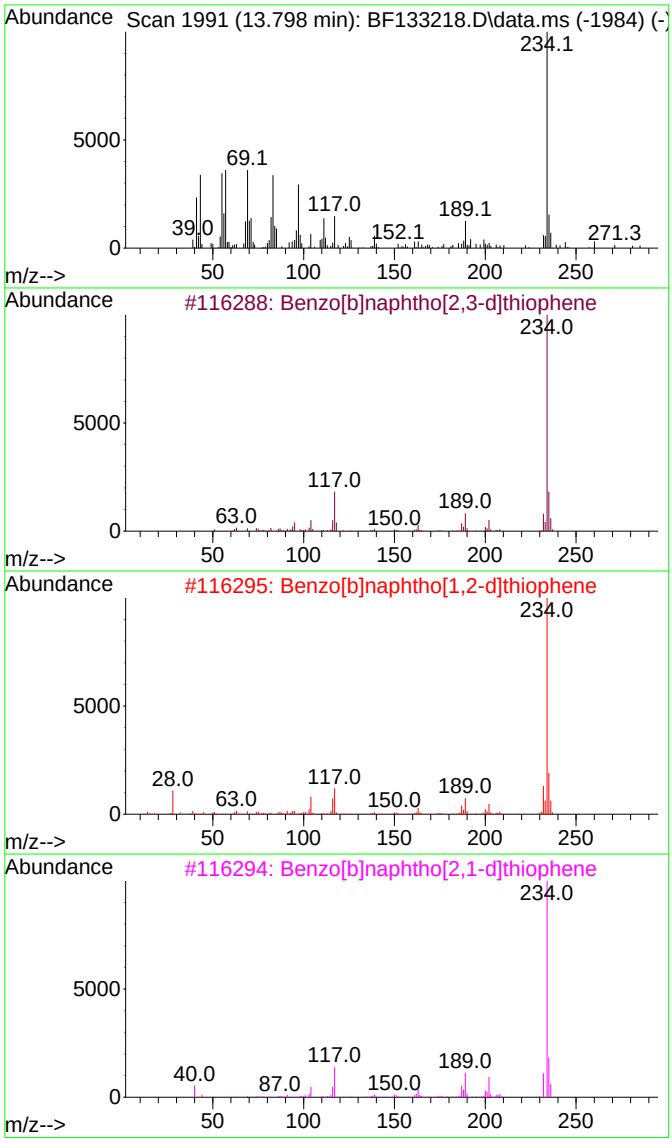
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

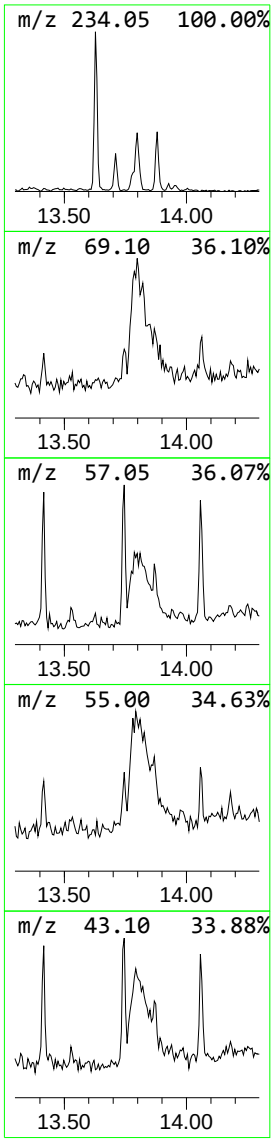
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzo[b]naphtho[2,3-d]thiop... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.798	3.13 ng	223020	Chrysene-d12	13.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]naphtho[2,3-d]thiophene	234	C16H10S	000243-46-9	90
2	Benzo[b]naphtho[1,2-d]thiophene	234	C16H10S	000205-43-6	81
3	Benzo[b]naphtho[2,1-d]thiophene	234	C16H10S	000239-35-0	76
4	Anthra(2,3-b)thiophene	234	C16H10S	022108-55-0	72
5	Phenanthro[4,3-b]thiophene	234	C16H10S	000195-68-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050323\
Data File : BF133218.D
Acq On : 03 May 2023 20:52
Operator : CG\JU
Sample : 02573-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-240

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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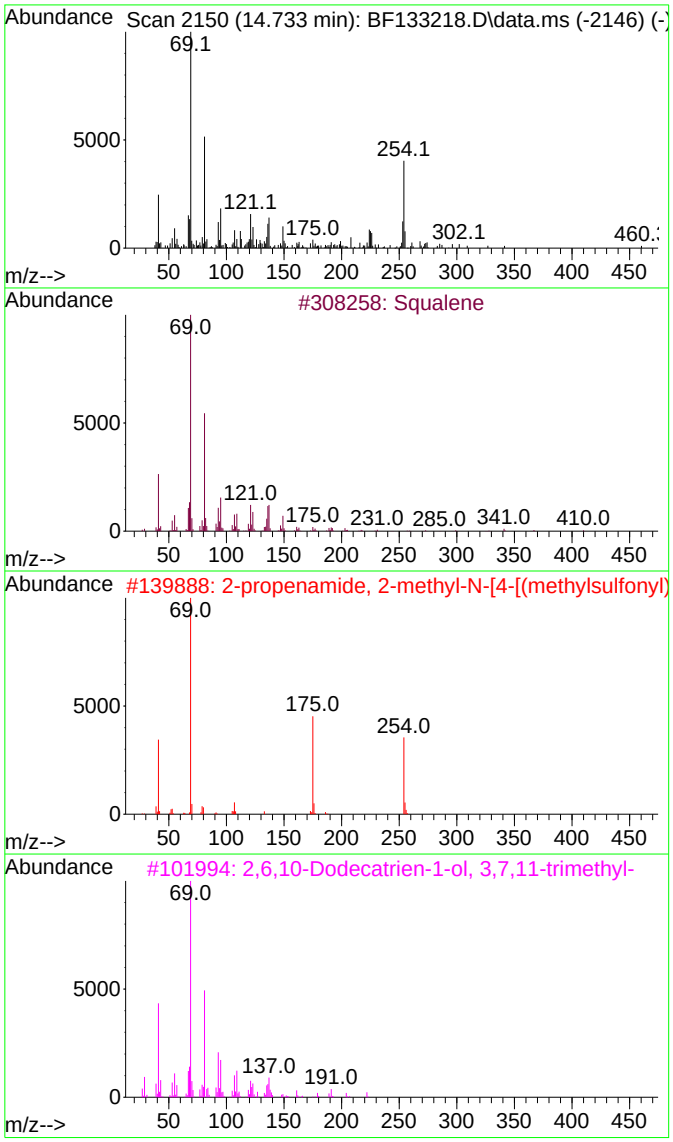
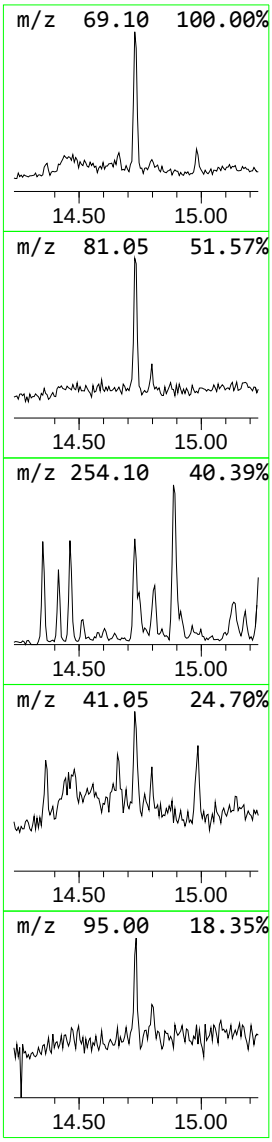
Peak Number 8 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.733	2.73 ng	142944	Perylene-d12	15.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	58
2	2-propenamide, 2-methyl-N-[4-[(m...	254	C11H14N2O3S	1000401-43-5	58
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	49
4	Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	47
5	5,9,13,17-Tetramethyl 4,8,12,16-...	332	C22H36O2	1000432-37-9	47





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Data File : BF133218.D
Acq On : 03 May 2023 20:52
Operator : CG\JU
Sample : 02573-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-240

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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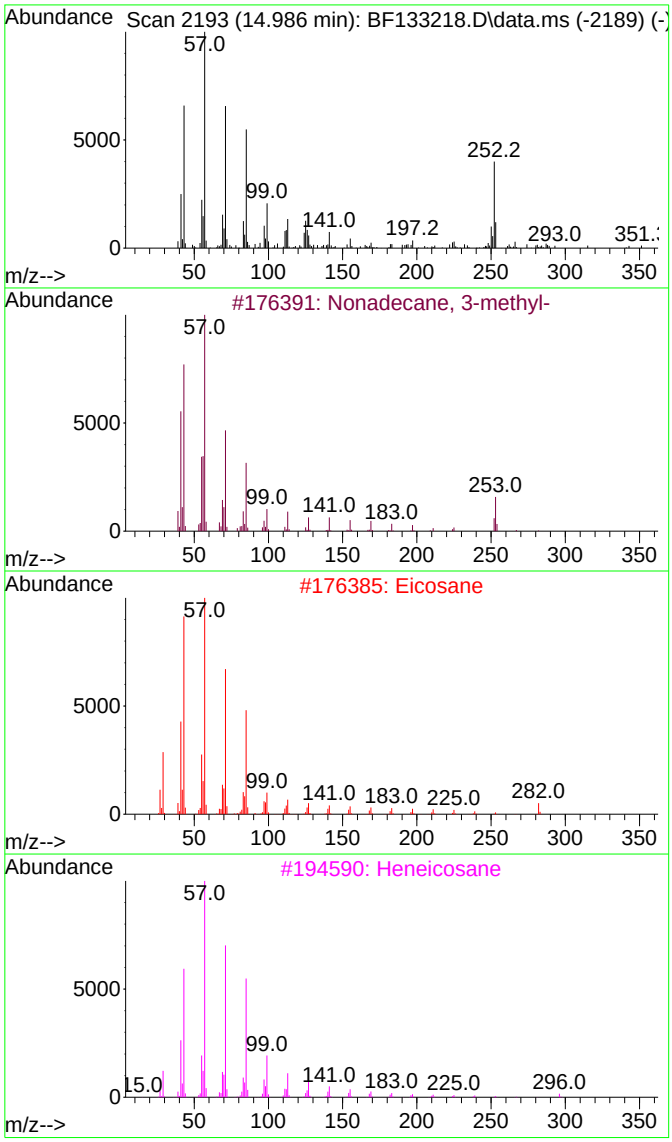
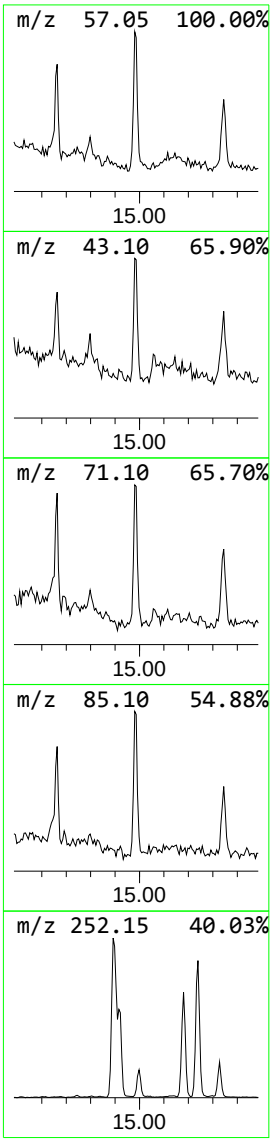
Peak Number 9 Nonadecane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.986	3.15 ng	164783	Perylene-d12	15.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 3-methyl-	282	C20H42	006418-45-7	58
2	Eicosane	282	C20H42	000112-95-8	55
3	Heneicosane	296	C21H44	000629-94-7	53
4	Hexacosane	366	C26H54	000630-01-3	53
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050323\
Data File : BF133218.D
Acq On : 03 May 2023 20:52
Operator : CG\JU
Sample : 02573-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-240

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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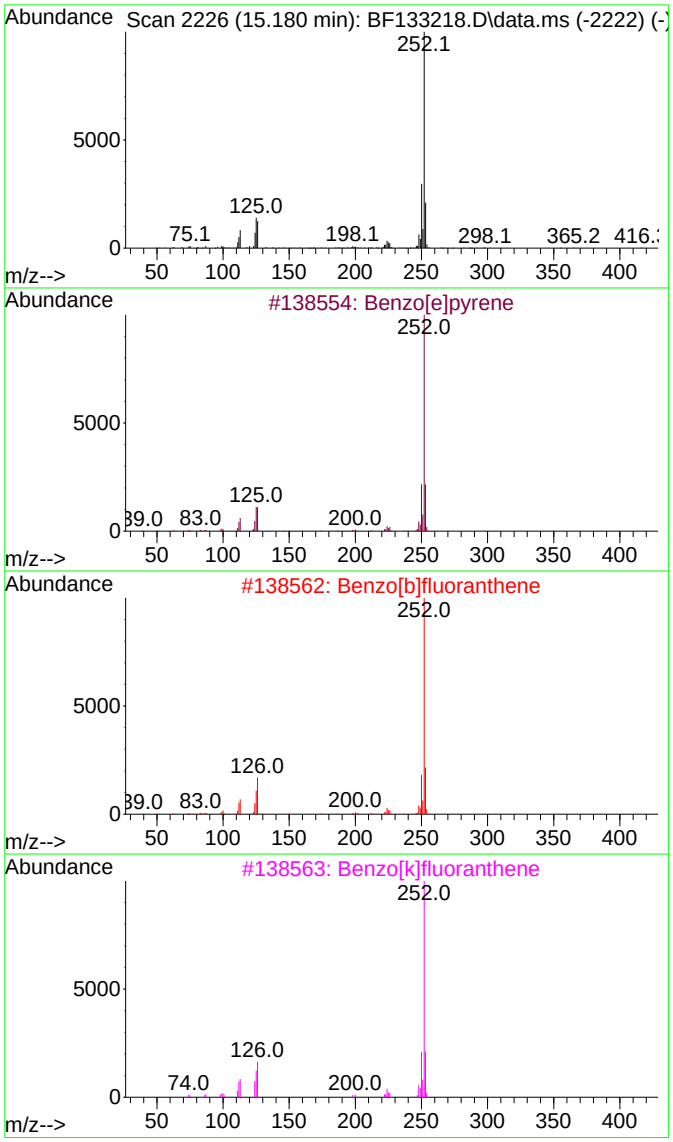
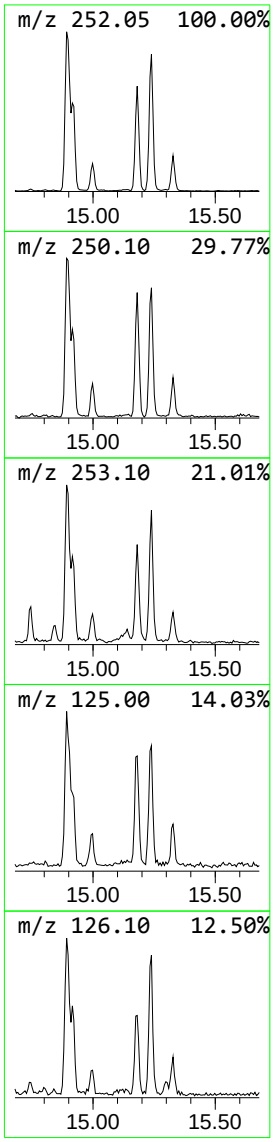
Peak Number 10 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.180	5.48 ng	286786	Perylene-d12	15.298

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	97
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050323\
Data File : BF133218.D
Acq On : 03 May 2023 20:52
Operator : CG\JU
Sample : 02573-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-240

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
Benzophenone	10.475	17.7	ng	1455480	3	9.763	1640450	20.0
Methanone, (1-h...	10.781	2.5	ng	185437	4	11.245	1507290	20.0
2-Propenoic aci...	10.869	3.6	ng	274607	4	11.245	1507290	20.0
Anthracene, 2-m...	11.775	3.4	ng	257433	4	11.245	1507290	20.0
4H-Cyclopenta[d...	11.857	3.3	ng	245898	4	11.245	1507290	20.0
11H-Benzo[b]flu...	13.075	2.2	ng	157809	5	13.880	1425610	20.0
Benzo[b]naphtho...	13.798	3.1	ng	223020	5	13.880	1425610	20.0
Squalene	14.733	2.7	ng	142944	6	15.298	1045990	20.0
Nonadecane, 3-m...	14.986	3.1	ng	164783	6	15.298	1045990	20.0
Benzo[e]pyrene	15.180	5.5	ng	286786	6	15.298	1045990	20.0