LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103123\
Data File : BF136058.D
Acq On : 31 Oct 2023 18:36
Operator : CG\JU
Sample : 04974-01
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-BF103023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136058.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	3	12	17	rVB	1050246	1568973	34.38%	3.480%
2	2.987	147	153	159	rVB	40483	66284	1.45%	0.147%
3	4.463	397	404	407	rBV	2625253	3186658	69.82%	7.067%
4	5.087	497	510	513	rBV	2666622	4564213	100.00%	10.122%
5	5.469	569	575	578	rBV	4014352	4053735	88.82%	8.990%
6	5.851	636	640	644	rVB	259756	206174	4.52%	0.457%
7	6.463	738	744	747	rBV	3452877	3808315	83.44%	8.446%
8	6.657	773	777	783	rBV	43169	53800	1.18%	0.119%
9	6.822	802	805	809	rBV	945245	783965	17.18%	1.739%
10	7.386	896	901	904	rBV	2527348	2425949	53.15%	5.380%
11	8.104	1019	1023	1026	rBV	1215868	936266	20.51%	2.076%
12	9.186	1203	1207	1210	rBV	4652512	3840177	84.14%	8.517%
13	9.863	1318	1322	1325	rBV	1108463	873355	19.13%	1.937%
14	9.892	1325	1327	1331	rVB	148026	112949	2.47%	0.250%
15	10.069	1353	1357	1360	rBV	65590	59064	1.29%	0.131%
16	10.410	1411	1415	1418	rBV	113311	86888	1.90%	0.193%
17	10.657	1452	1457	1460	rBV	2477721	2312709	50.67%	5.129%
18	11.251	1555	1558	1565	rVB	63717	61186	1.34%	0.136%
19	11.357	1572	1576	1578	rBV	1000194	943737	20.68%	2.093%
20	11.380	1578	1580	1583	rVV	1160672	883299	19.35%	1.959%
21	11.427	1585	1588	1591	rVB	269597	223033	4.89%	0.495%
22	11.586	1609	1615	1618	rBV	107950	105866	2.32%	0.235%
23	11.857	1656	1661	1664	rBV	104045	103187	2.26%	0.229%
24	11.892	1664	1667	1671	rVV2	343832	343664	7.53%	0.762%
25	11.933	1671	1674	1677	rVV2	65145	71238	1.56%	0.158%
26	11.968	1677	1680	1683	rVV	187570	211493	4.63%	0.469%
27	11.992	1683	1684	1689	rVB	83230	57954	1.27%	0.129%
28	12.157	1709	1712	1714	rBV	100831	89725	1.97%	0.199%
29	12.180	1714	1716	1720	rVB	87150	73358	1.61%	0.163%
30	12.416	1752	1756	1758	rBV	65863	72047	1.58%	0.160%
31	12.498	1767	1770	1775	rVB4	58528	68222	1.49%	0.151%
32	12.574	1779	1783	1787	rVV	1595967	1353746	29.66%	3.002%
33	12.686	1799	1802	1807	rBV4	60719	78503	1.72%	0.174%
34	12.727	1807	1809	1816	rVB	49814	53282	1.17%	0.118%
35	12.804	1816	1822	1826	rBV	1277190	1350963	29.60%	2.996%
36	12.857	1828	1831	1835	rVB2	53087	72969	1.60%	0.162%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103123\
Data File : BF136058.D
Acq On : 31 Oct 2023 18:36
Operator : CG\JU
Sample : 04974-01
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-BF103023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.927	1839	1843	1844	rBV	81454	72072	1.58%	0.160%
38	12.957	1844	1848	1852	rVV	4124806	4057204	88.89%	8.998%
39	13.027	1855	1860	1863	rBV3	64175	113834	2.49%	0.252%
40	13.110	1871	1874	1876	rBV2	48349	56555	1.24%	0.125%
41	13.139	1876	1879	1882	rVB	148812	144767	3.17%	0.321%
42	13.204	1886	1890	1892	rBV2	124326	104397	2.29%	0.232%
43	13.239	1892	1896	1899	rBV	113170	106704	2.34%	0.237%
44	13.363	1915	1917	1921	rBV2	59494	55839	1.22%	0.124%
45	13.545	1941	1948	1950	rBV5	43114	71513	1.57%	0.159%
46	13.645	1962	1965	1970	rVB	94108	97771	2.14%	0.217%
47	13.757	1980	1984	1987	rBV2	97199	126380	2.77%	0.280%
48	13.786	1987	1989	1991	rVV	89706	79052	1.73%	0.175%
49	13.810	1991	1993	1997	rVV3	86090	111625	2.45%	0.248%
50	13.851	1998	2000	2003	rVV	88205	80724	1.77%	0.179%
51	13.904	2005	2009	2019	rVB4	60635	187925	4.12%	0.417%
52	14.010	2022	2027	2030	rBV2	1201632	1613393	35.35%	3.578%
53	14.039	2030	2032	2034	rVB	577743	407949	8.94%	0.905%
54	14.115	2043	2045	2048	rVB	134598	110891	2.43%	0.246%
55	14.404	2091	2094	2096	rVV	72916	63564	1.39%	0.141%
56	14.433	2097	2099	2102	rVB2	51970	46240	1.01%	0.103%
57	14.498	2107	2110	2113	rBV5	59296	85473	1.87%	0.190%
58	15.062	2202	2206	2210	rBV	360804	591209	12.95%	1.311%
59	15.174	2222	2225	2229	rVB2	81095	84271	1.85%	0.187%
60	15.374	2256	2259	2265	rVB	196377	236815	5.19%	0.525%
61	15.439	2266	2270	2276	rVB	284565	329648	7.22%	0.731%
62	15.504	2277	2281	2285	rBV	547521	682790	14.96%	1.514%
63	17.009	2533	2537	2548	rVB3	93637	214339	4.70%	0.475%

Sum of corrected areas: 45089890

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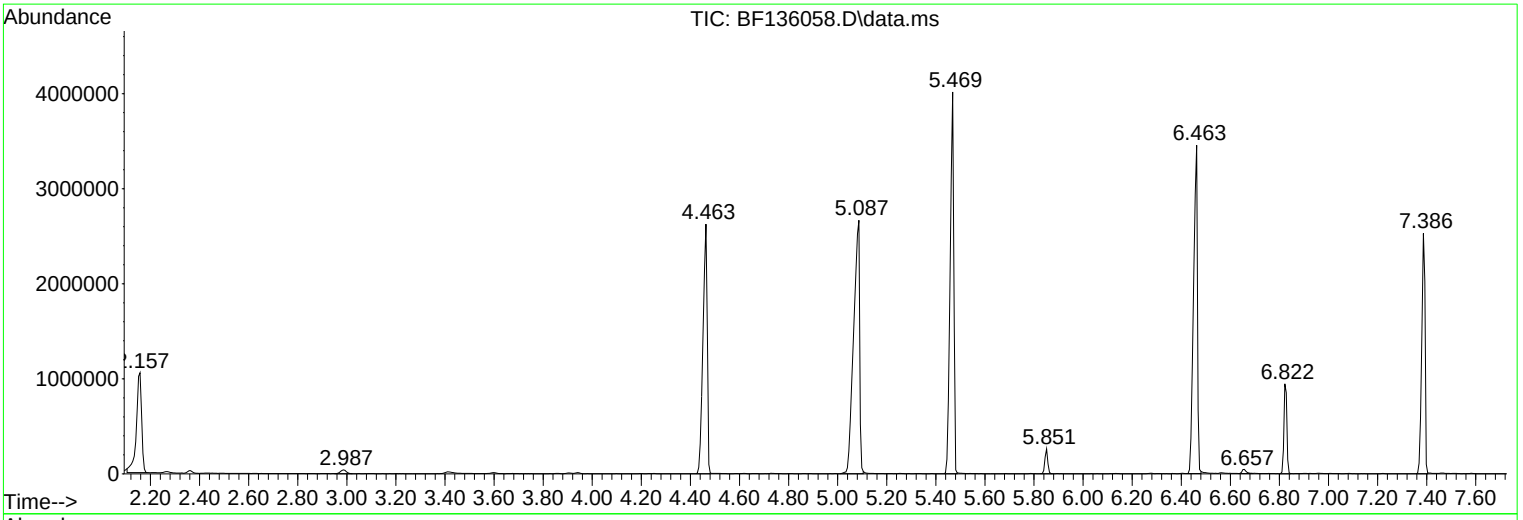
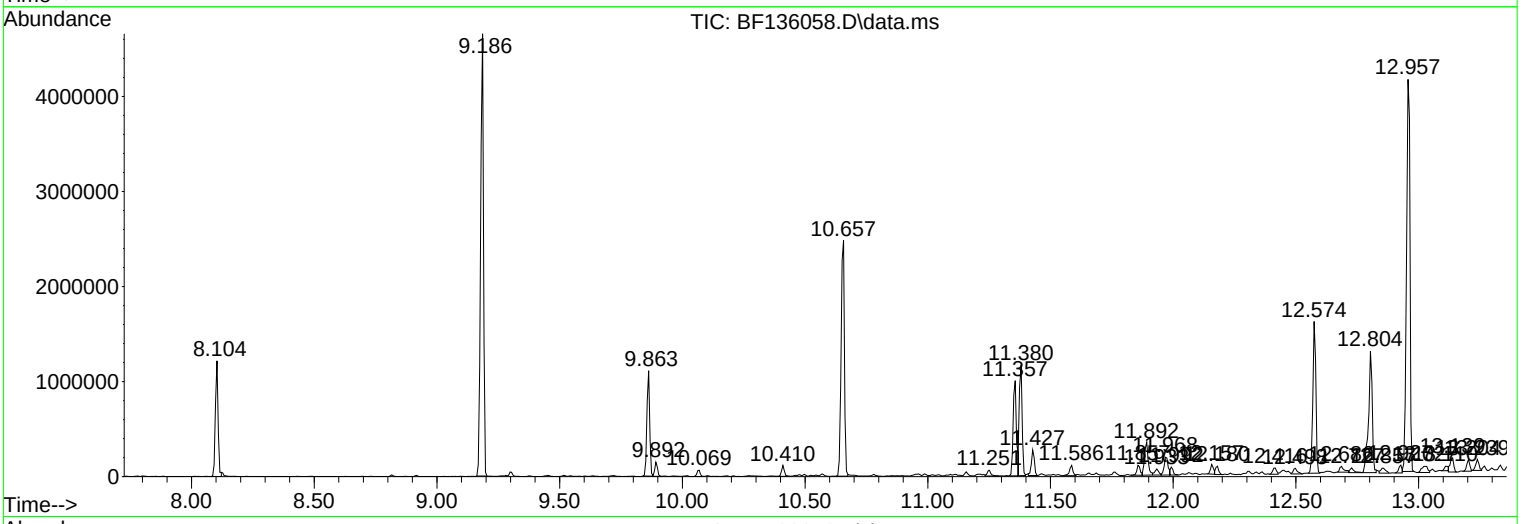
Misc :
ALS Vial : 16 Sample Multiplier: 1

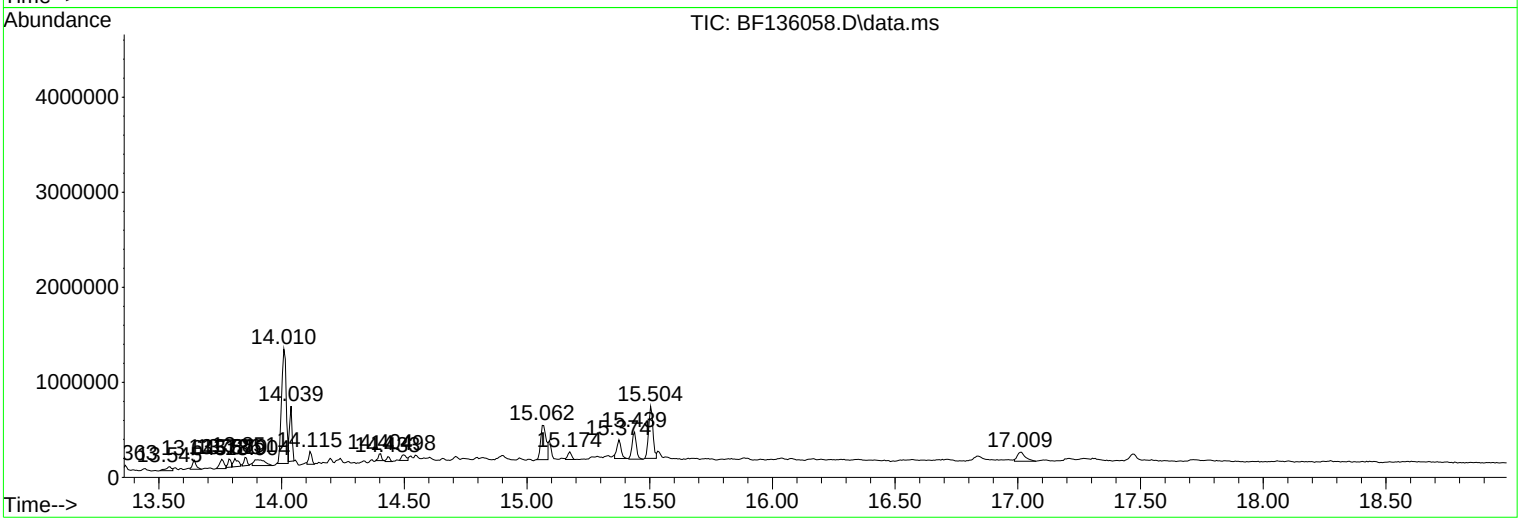
Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.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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Data File : BF136058.D
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Operator : CG\JU
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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

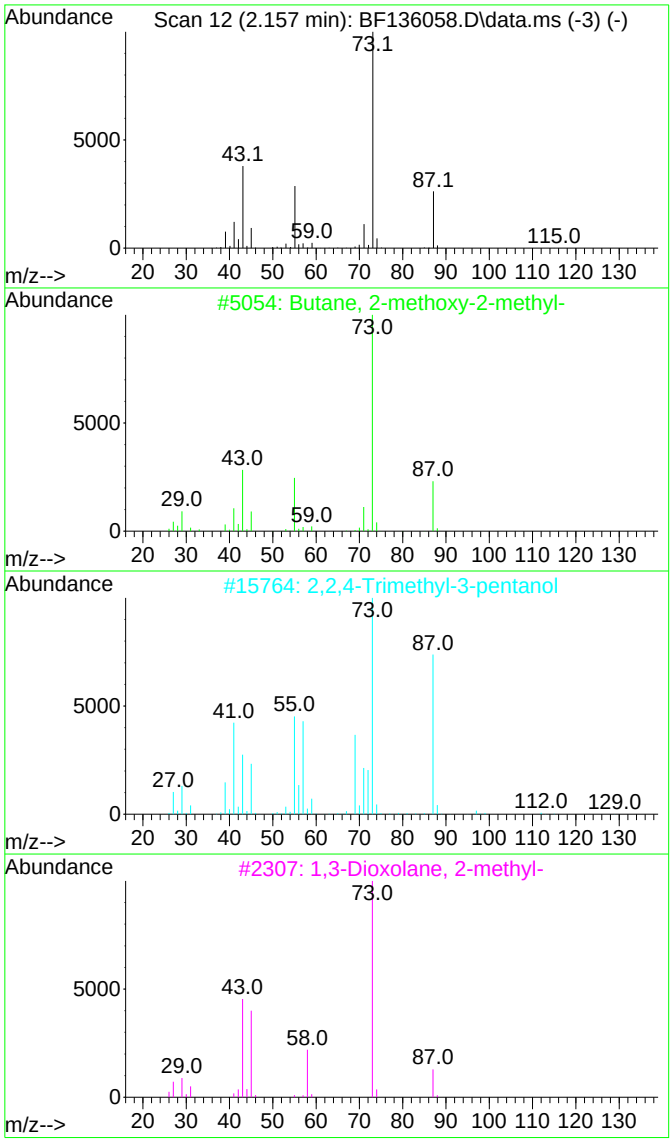
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

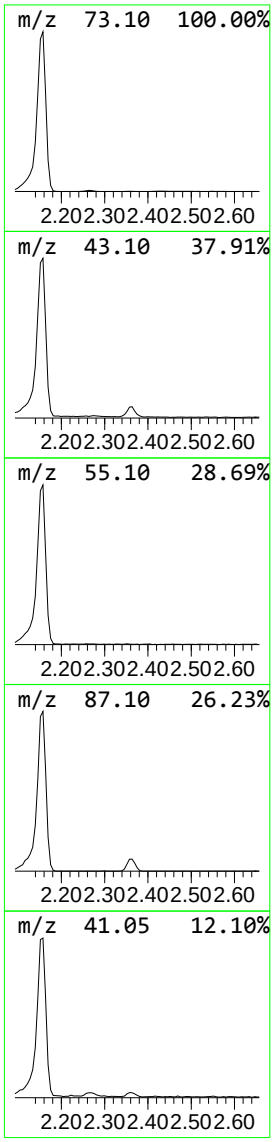
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	40.03 ng	1568970	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103123\
Data File : BF136058.D
Acq On : 31 Oct 2023 18:36
Operator : CG\JU
Sample : 04974-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

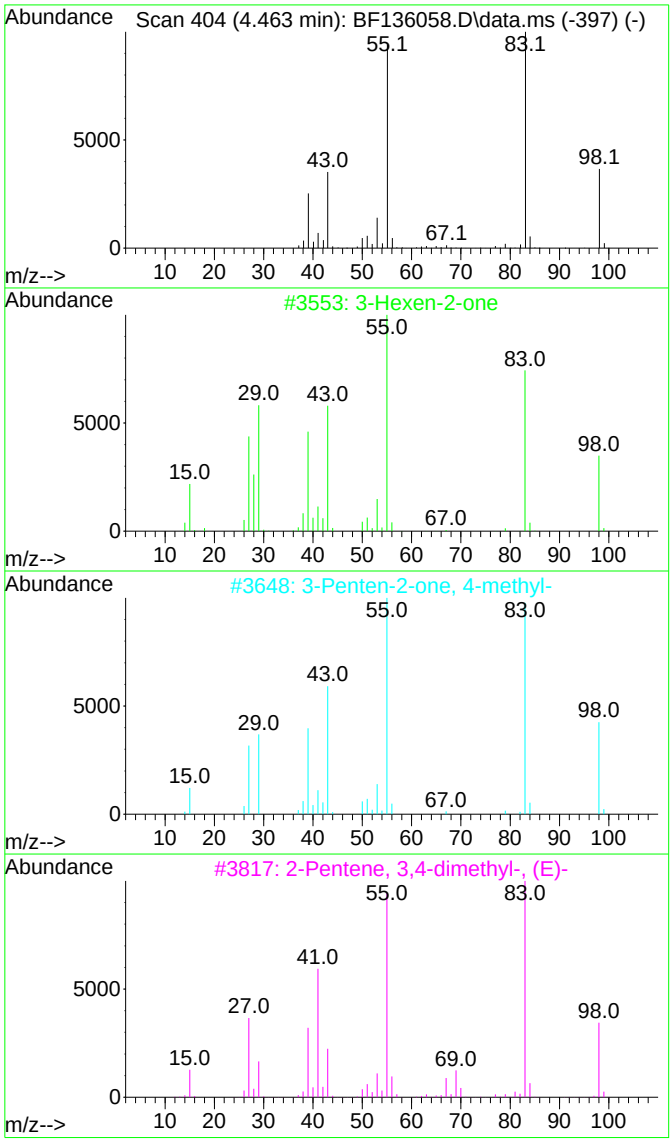
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

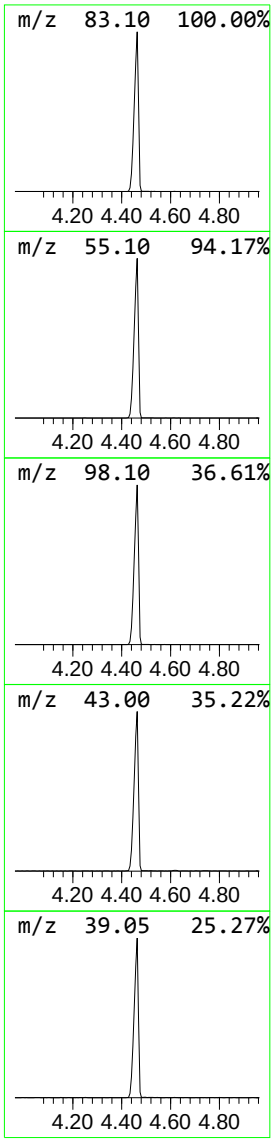
****

Peak Number 2 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.463	81.30 ng	3186660	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103123\
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Acq On : 31 Oct 2023 18:36
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Sample : 04974-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

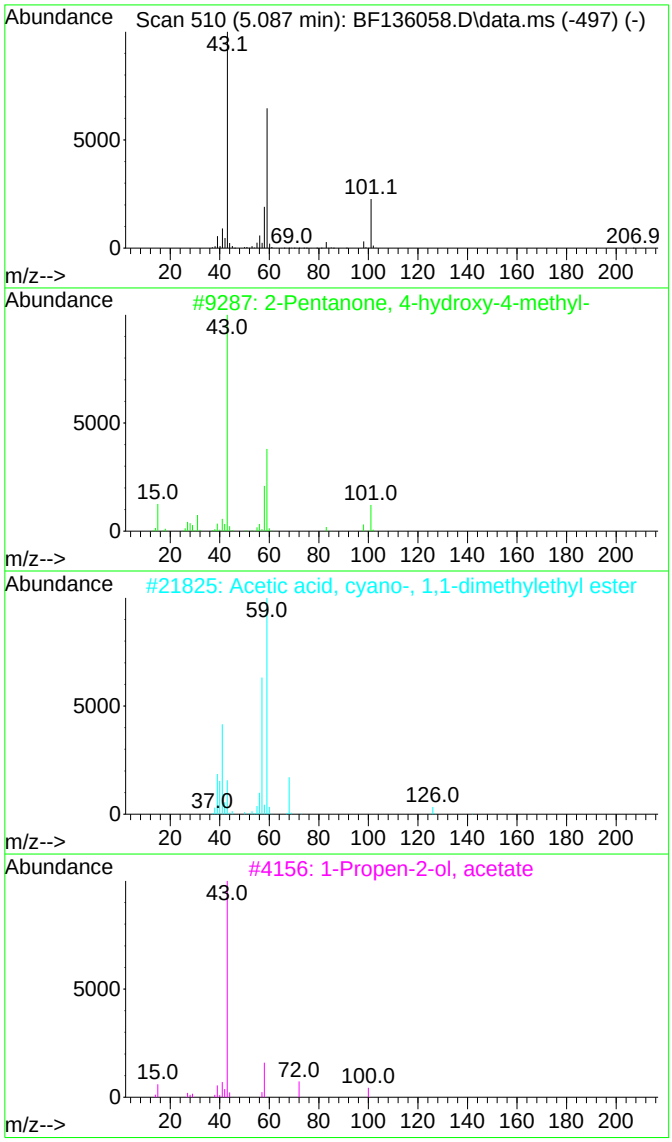
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

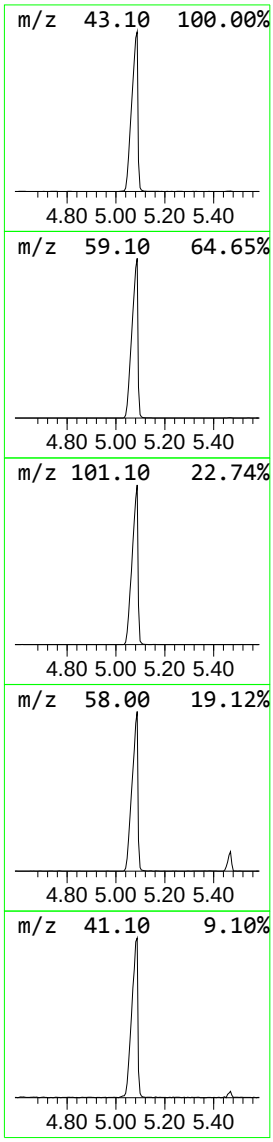
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	116.44 ng	4564210	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	Acetone	58	C3H6O	000067-64-1	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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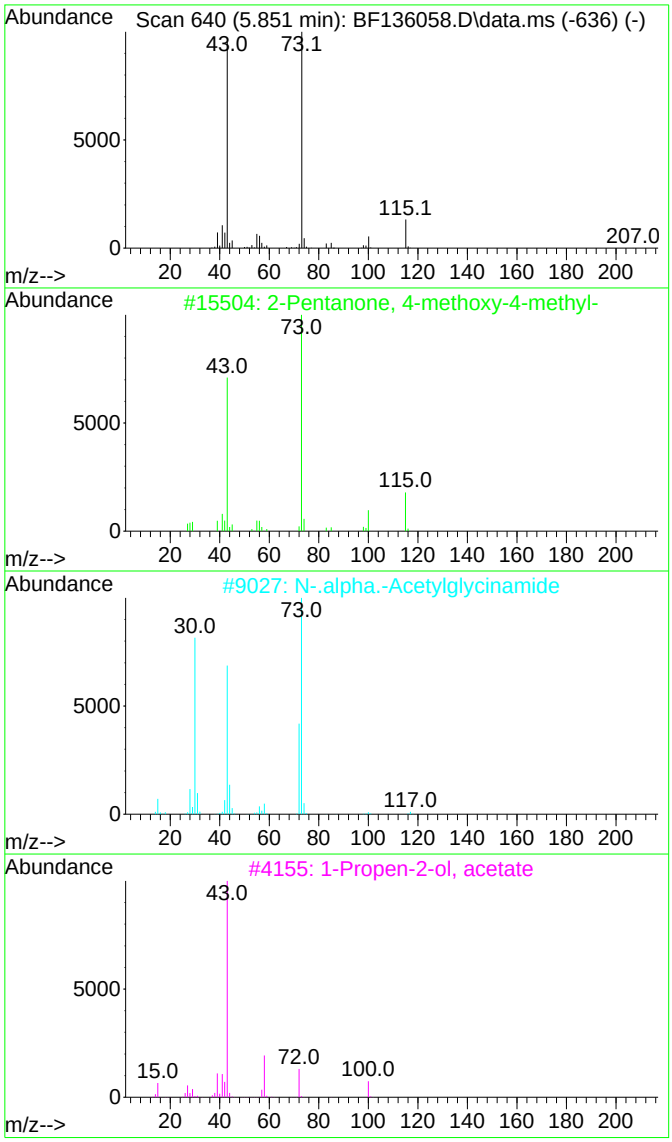
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

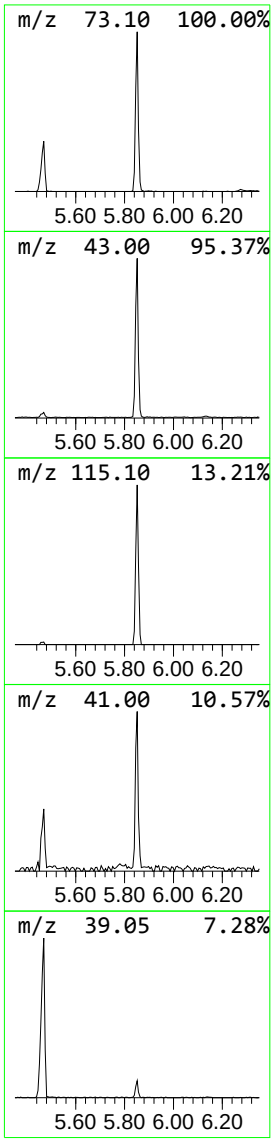
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.851	5.26 ng	206174	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103123\
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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-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

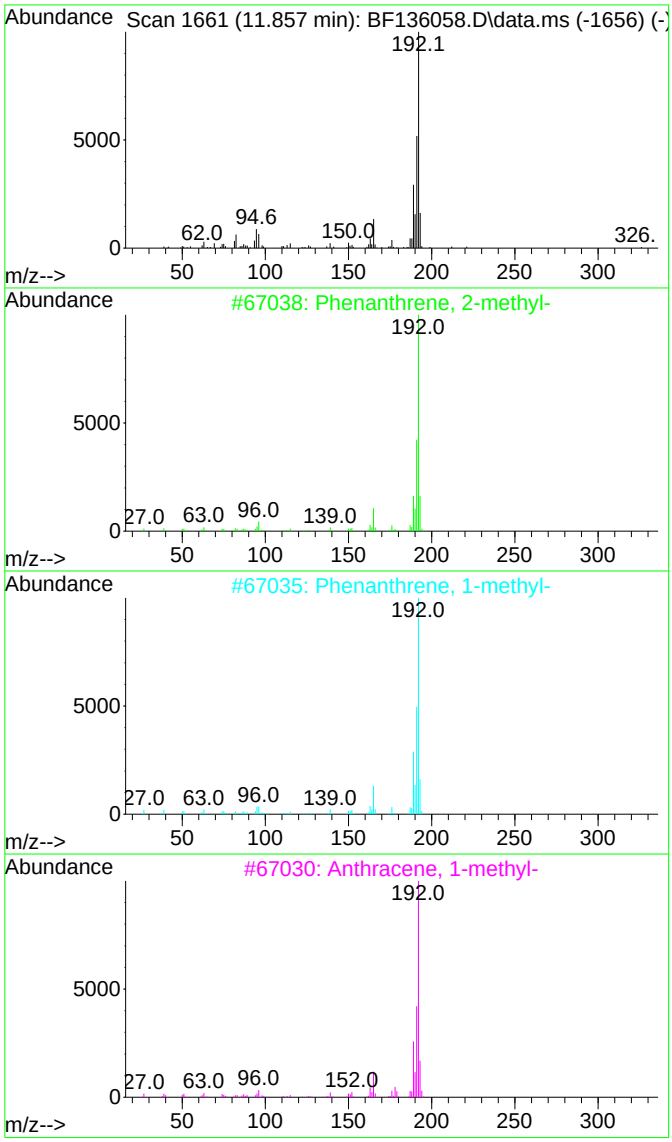
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

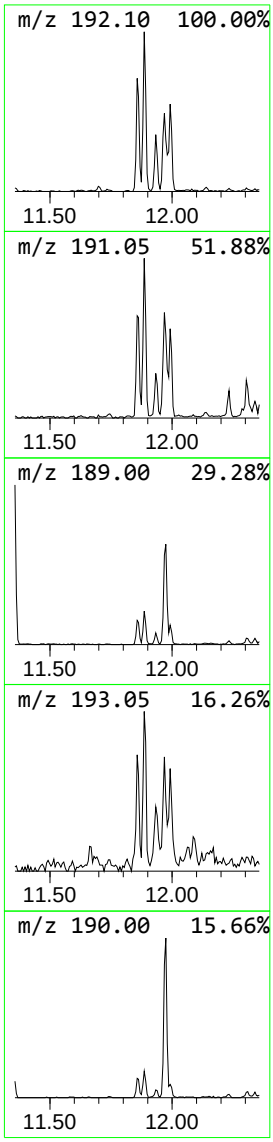
****

Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	2.19 ng	103187	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	93
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91





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Data File : BF136058.D
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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-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

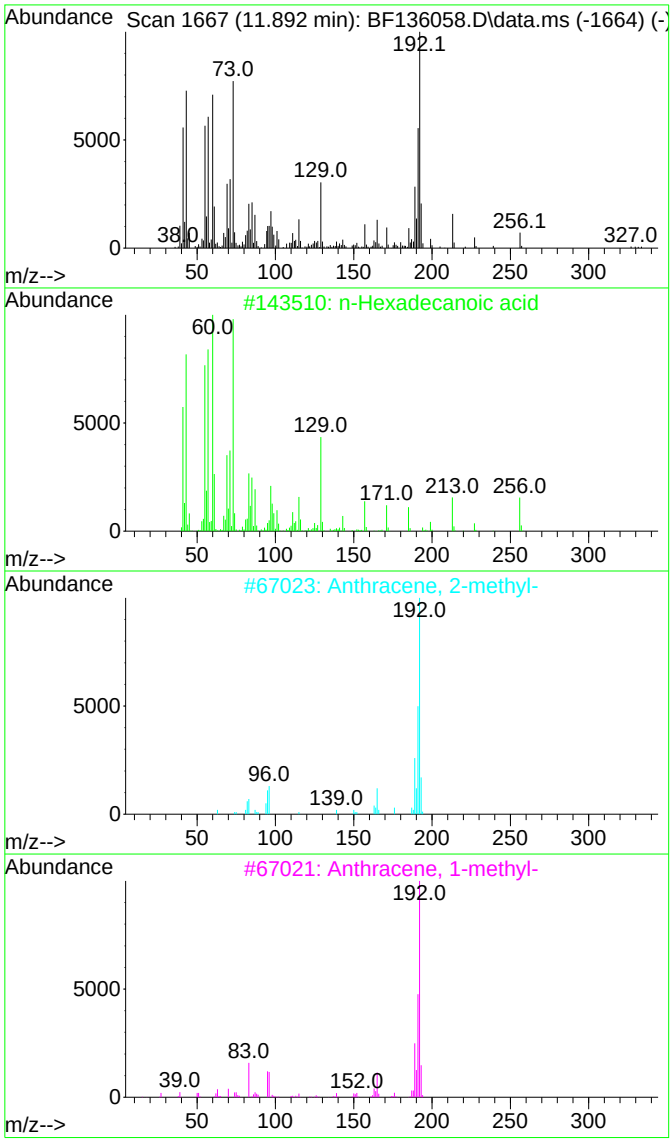
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

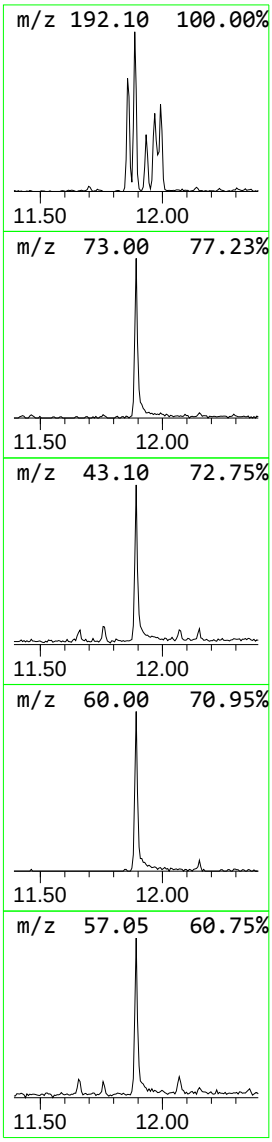
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	7.28 ng	343664	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	94
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103123\
Data File : BF136058.D
Acq On : 31 Oct 2023 18:36
Operator : CG\JU
Sample : 04974-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

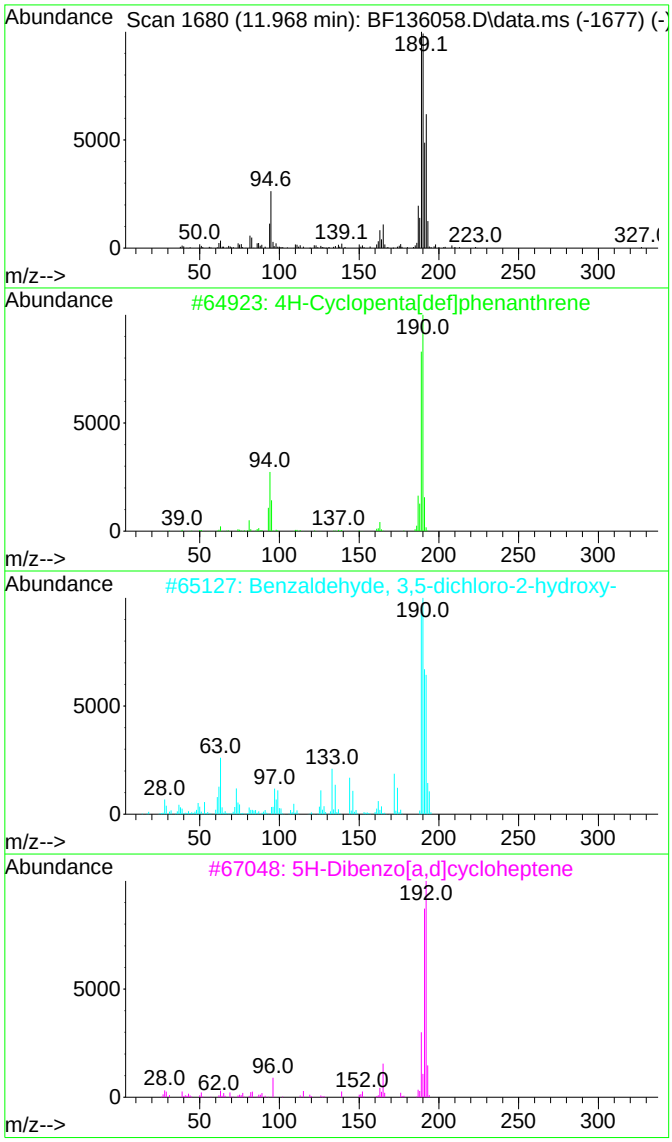
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

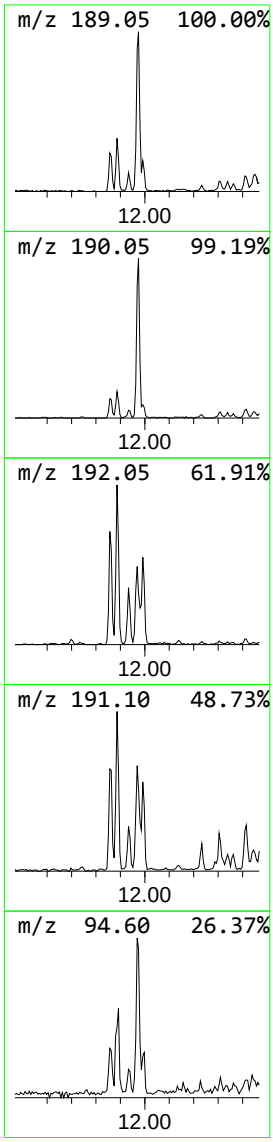
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	4.48 ng	211493	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	92
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	72
3	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	25
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	25
5	Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	25





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Data File : BF136058.D
Acq On : 31 Oct 2023 18:36
Operator : CG\JU
Sample : 04974-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.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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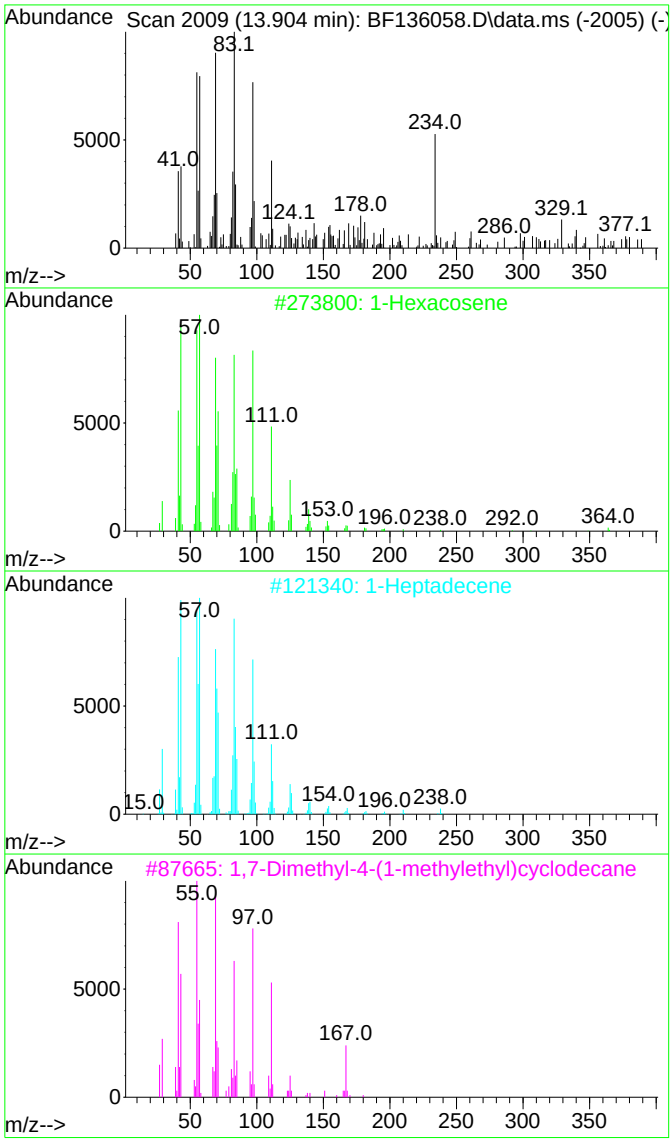
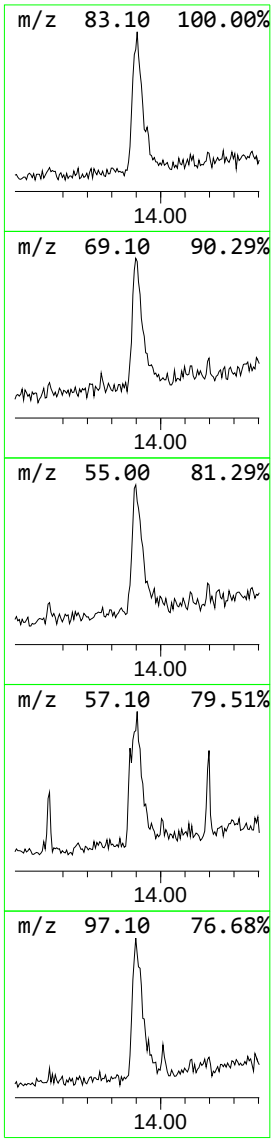
Peak Number 8 1-Hexacosene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	2.33 ng	187925	Chrysene-d12	14.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	64
2	1-Heptadecene	238	C17H34	006765-39-5	59
3	1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	50
4	3-Heptene, 4-propyl-	140	C10H20	004485-13-6	43
5	6-Bromo-2,2-dimethylcyclohexanone	204	C8H13BrO	021690-26-6	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103123\
Data File : BF136058.D
Acq On : 31 Oct 2023 18:36
Operator : CG\JU
Sample : 04974-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.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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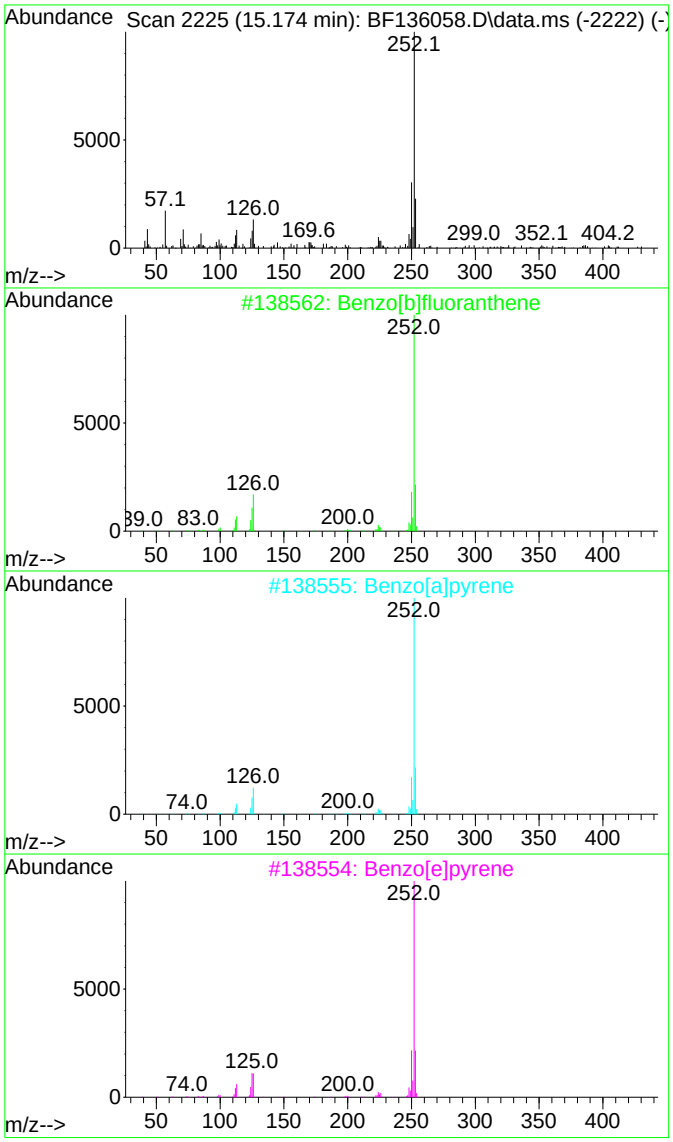
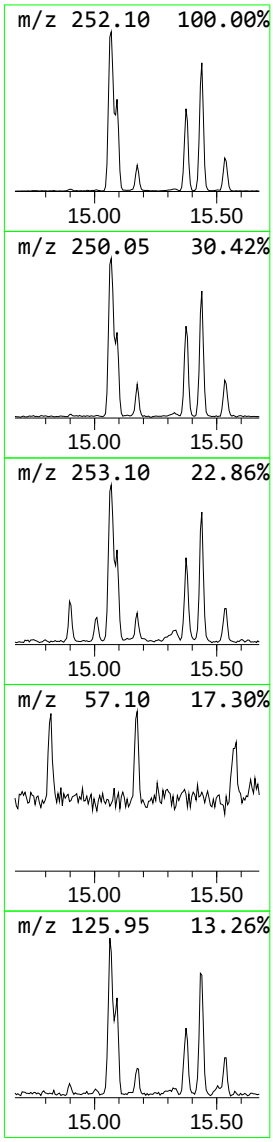
Peak Number 9 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	2.47 ng	84271	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
2	Benzo[a]pyrene	252	C20H12	000050-32-8	94
3	Benzo[e]pyrene	252	C20H12	000192-97-2	94
4	1,1'-Binaphthalene, 2,2'-dibromo-	410	C20H12Br2	074866-28-7	91
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	89





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103123\
Data File : BF136058.D
Acq On : 31 Oct 2023 18:36
Operator : CG\JU
Sample : 04974-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.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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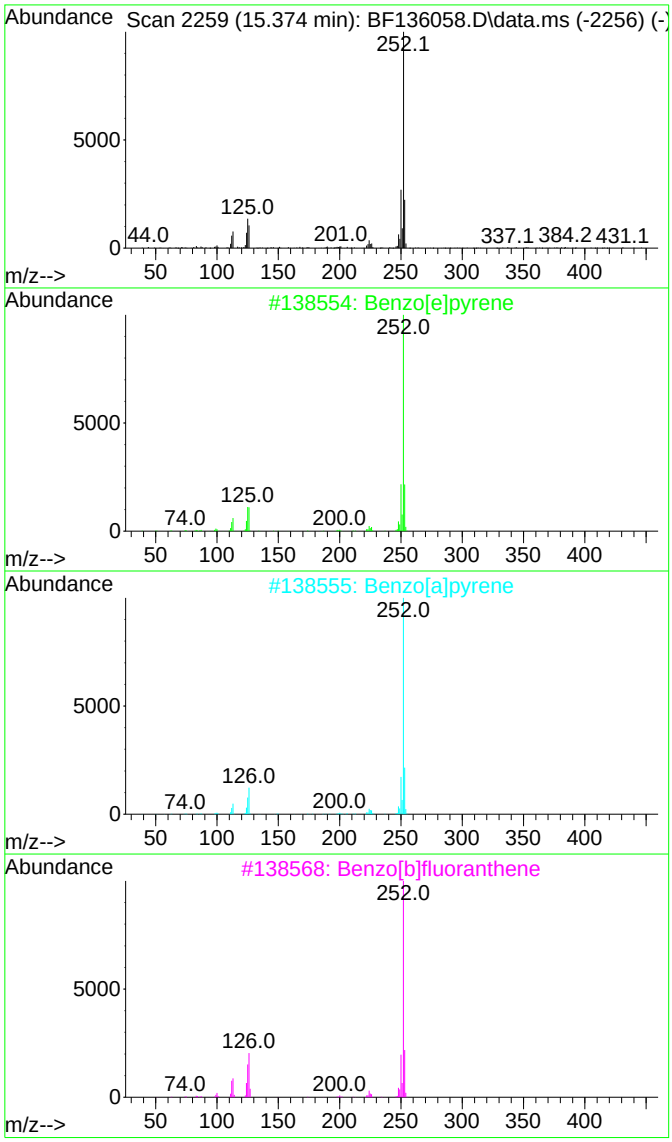
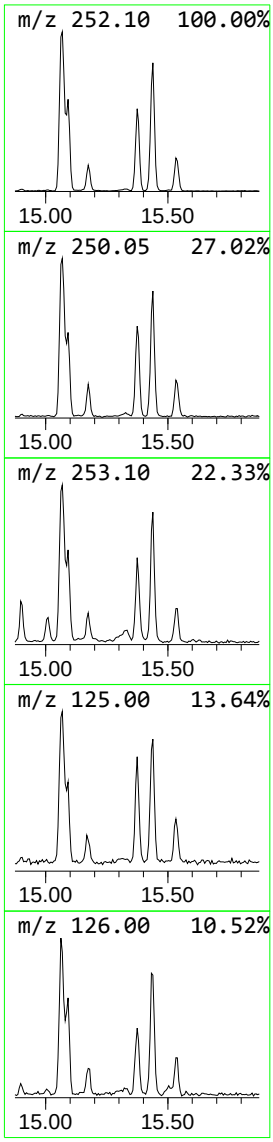
Peak Number 10 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.374	6.94 ng	236815	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	98
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
5	Perylene	252	C20H12	000198-55-0	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103123\
Data File : BF136058.D
Acq On : 31 Oct 2023 18:36
Operator : CG\JU
Sample : 04974-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.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...	2.157	40.0	ng	1568970	1	6.822	783965	20.0
3-Hexen-2-one	4.463	81.3	ng	3186660	1	6.822	783965	20.0
2-Pentanone, 4-...	5.087	116.4	ng	4564210	1	6.822	783965	20.0
2-Pentanone, 4-...	5.851	5.3	ng	206174	1	6.822	783965	20.0
Phenanthrene, 2...	11.857	2.2	ng	103187	4	11.357	943737	20.0
n-Hexadecanoic ...	11.892	7.3	ng	343664	4	11.357	943737	20.0
4H-Cyclopenta[d...	11.969	4.5	ng	211493	4	11.357	943737	20.0
1-Hexacosene	13.904	2.3	ng	187925	5	14.015	1613390	20.0
Benzo[e]pyrene	15.174	2.5	ng	84271	6	15.504	682790	20.0
Perylene	15.374	6.9	ng	236815	6	15.504	682790	20.0