LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139332.D
Acq On : 11 Sep 2024 18:12
Operator : RC/JU
Sample : P3929-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11930

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-BF090424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139332.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	10	19	26	rBV	1344994	2145464	97.11%	10.484%
2	5.110	503	513	525	rBB	83084	131770	5.96%	0.644%
3	5.504	574	580	585	rBV	1352346	1835885	83.09%	8.971%
4	6.510	744	751	756	rBV	1380156	1954330	88.45%	9.550%
5	6.881	809	814	819	rVB	328359	405553	18.36%	1.982%
6	7.445	904	910	915	rBV	948969	1261661	57.10%	6.165%
7	7.698	949	953	957	rBB	36851	44279	2.00%	0.216%
8	8.163	1027	1032	1037	rBV	411325	507016	22.95%	2.478%
9	9.239	1209	1215	1220	rBV	1763259	2209423	100.00%	10.797%
10	9.916	1325	1330	1335	rBV	647056	823609	37.28%	4.025%
11	10.633	1444	1452	1459	rBV	168397	210607	9.53%	1.029%
12	10.704	1459	1464	1479	rBV	1236275	1602849	72.55%	7.833%
13	11.404	1578	1583	1591	rBV	545974	736351	33.33%	3.598%
14	11.474	1591	1595	1599	rBV	54232	74666	3.38%	0.365%
15	11.933	1664	1673	1678	rBV	397334	572103	25.89%	2.796%
16	12.016	1684	1687	1696	rVB2	45472	83609	3.78%	0.409%
17	12.451	1757	1761	1765	rBV	18025	24122	1.09%	0.118%
18	12.539	1773	1776	1781	rVB	17792	22353	1.01%	0.109%
19	12.616	1784	1789	1795	rBV	390746	508160	23.00%	2.483%
20	12.715	1802	1806	1813	rBV	54285	80169	3.63%	0.392%
21	12.845	1820	1828	1833	rBV2	223819	361512	16.36%	1.767%
22	12.892	1833	1836	1843	rVB3	23043	34002	1.54%	0.166%
23	12.992	1844	1853	1858	rBV	1593260	2055001	93.01%	10.042%
24	13.063	1859	1865	1870	rBV3	28771	52059	2.36%	0.254%
25	13.168	1876	1883	1888	rVB2	58557	102333	4.63%	0.500%
26	13.239	1888	1895	1898	rBV	55431	82109	3.72%	0.401%
27	13.274	1898	1901	1904	rVB2	23162	28020	1.27%	0.137%
28	13.674	1967	1969	1975	rVB	25596	35324	1.60%	0.173%
29	13.792	1984	1989	1991	rBV3	36434	51634	2.34%	0.252%
30	13.821	1991	1994	2000	rVV3	29341	74774	3.38%	0.365%
31	13.886	2001	2005	2022	rVV5	121663	322319	14.59%	1.575%
32	14.039	2024	2031	2046	rVV3	493856	1044119	47.26%	5.102%
33	14.515	2108	2112	2115	rBV3	23585	37759	1.71%	0.185%
34	14.562	2116	2120	2126	rVB3	30628	53547	2.42%	0.262%
35	14.674	2135	2139	2143	rBV	26587	42317	1.92%	0.207%
36	14.898	2173	2177	2185	rVB	77283	105892	4.79%	0.517%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139332.D
Acq On : 11 Sep 2024 18:12
Operator : RC/JU
Sample : P3929-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11930

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-BF090424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.080	2204	2208	2219	rVB2	66554	161983	7.33%	0.792%
38	15.386	2256	2260	2266	rVB	26187	43795	1.98%	0.214%
39	15.445	2266	2270	2276	rVV	33545	53400	2.42%	0.261%
40	15.515	2276	2282	2294	rVB	270323	435187	19.70%	2.127%
41	16.980	2527	2531	2540	rVB2	13216	28443	1.29%	0.139%
42	17.421	2603	2606	2613	rVB	12459	24210	1.10%	0.118%

Sum of corrected areas: 20463718

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139332.D
Acq On : 11 Sep 2024 18:12
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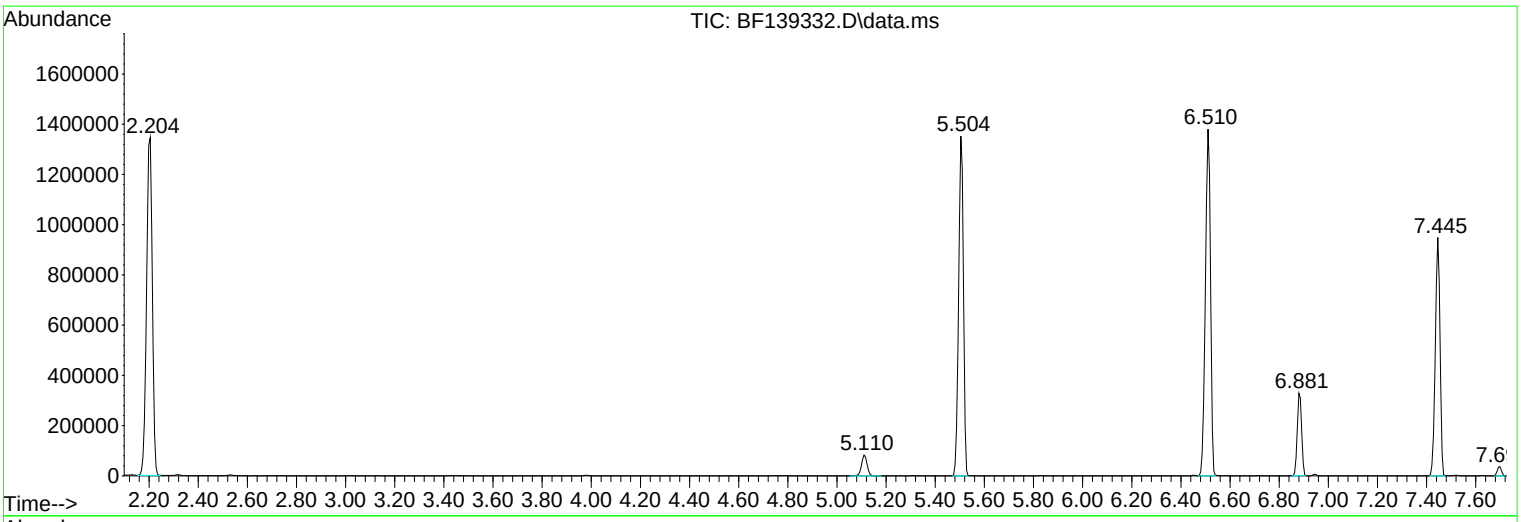
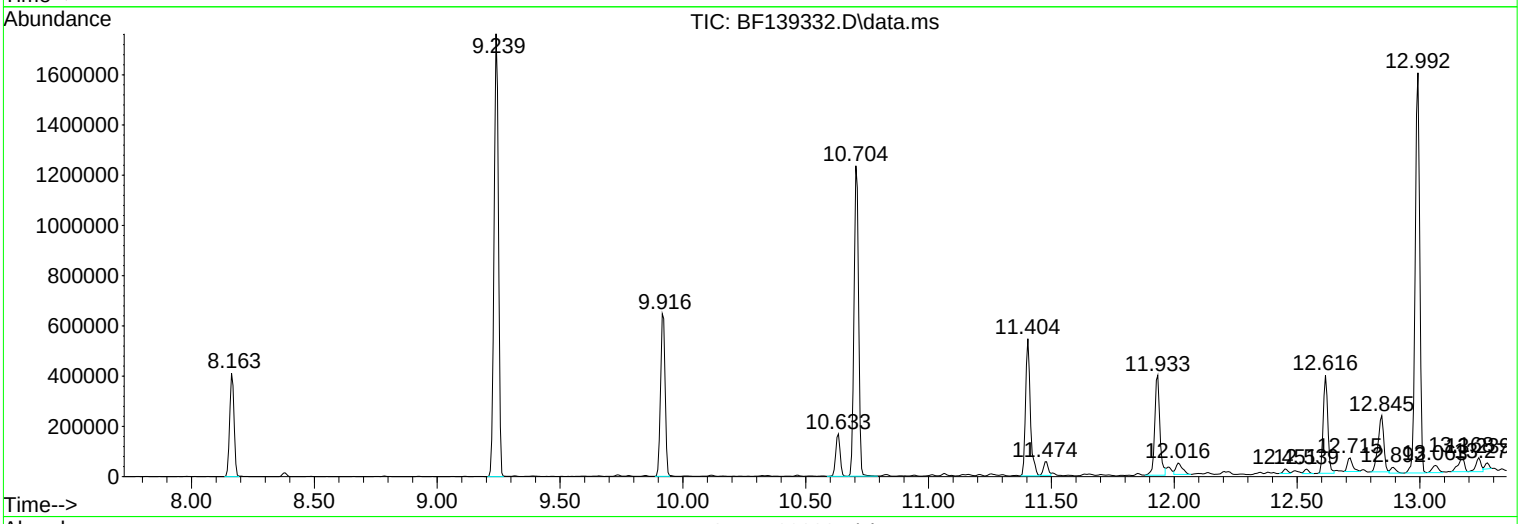
Misc :
ALS Vial : 19 Sample Multiplier: 1

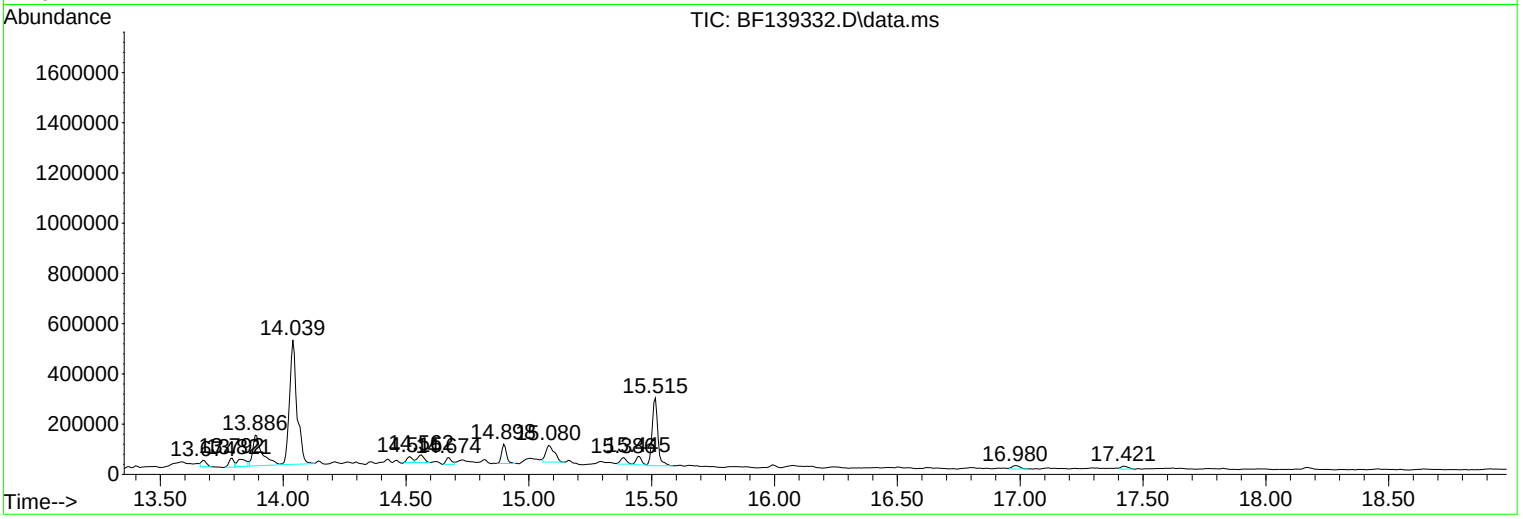
Instrument :
BNA_F
ClientSampleId :
72-11930

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.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\BF091124\
Data File : BF139332.D
Acq On : 11 Sep 2024 18:12
Operator : RC/JU
Sample : P3929-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

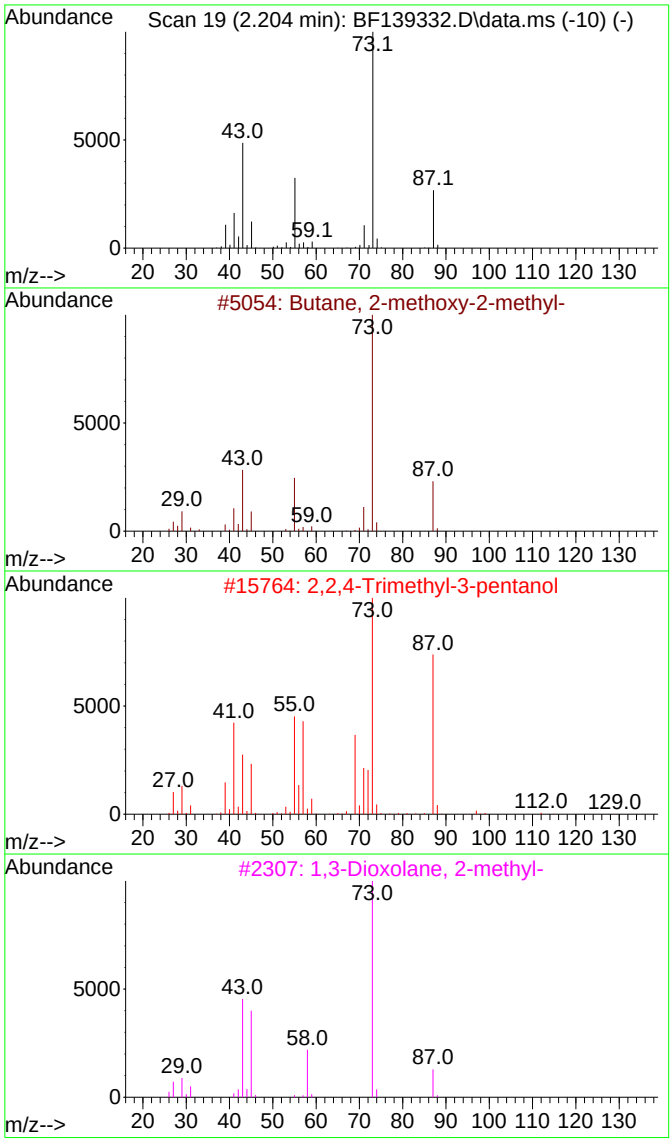
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

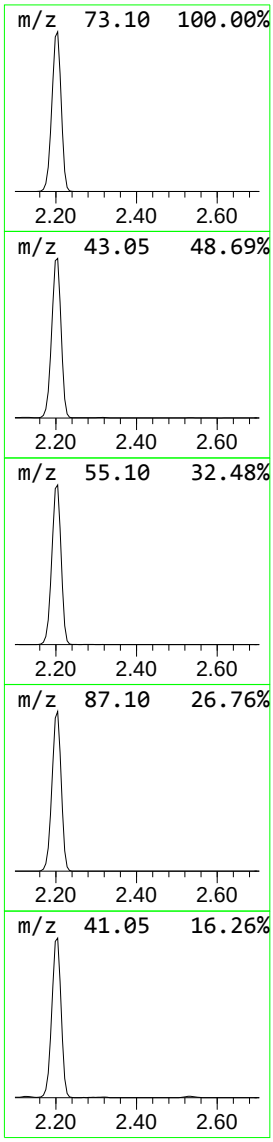
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	105.80 ng	2145460	1,4-Dichlorobenzene-d4	6.881

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139332.D
Acq On : 11 Sep 2024 18:12
Operator : RC/JU
Sample : P3929-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11930

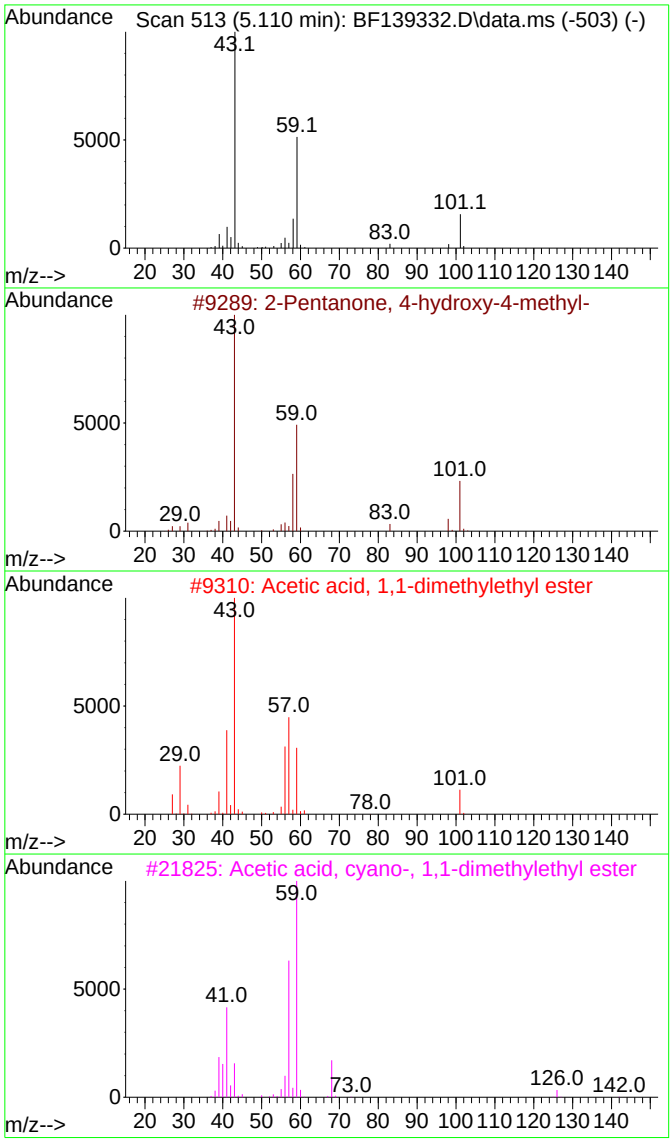
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

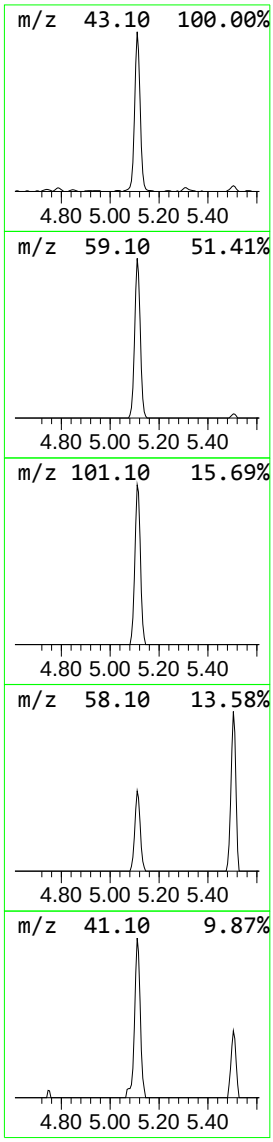
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	6.50 ng	131770	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139332.D
Acq On : 11 Sep 2024 18:12
Operator : RC/JU
Sample : P3929-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11930

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

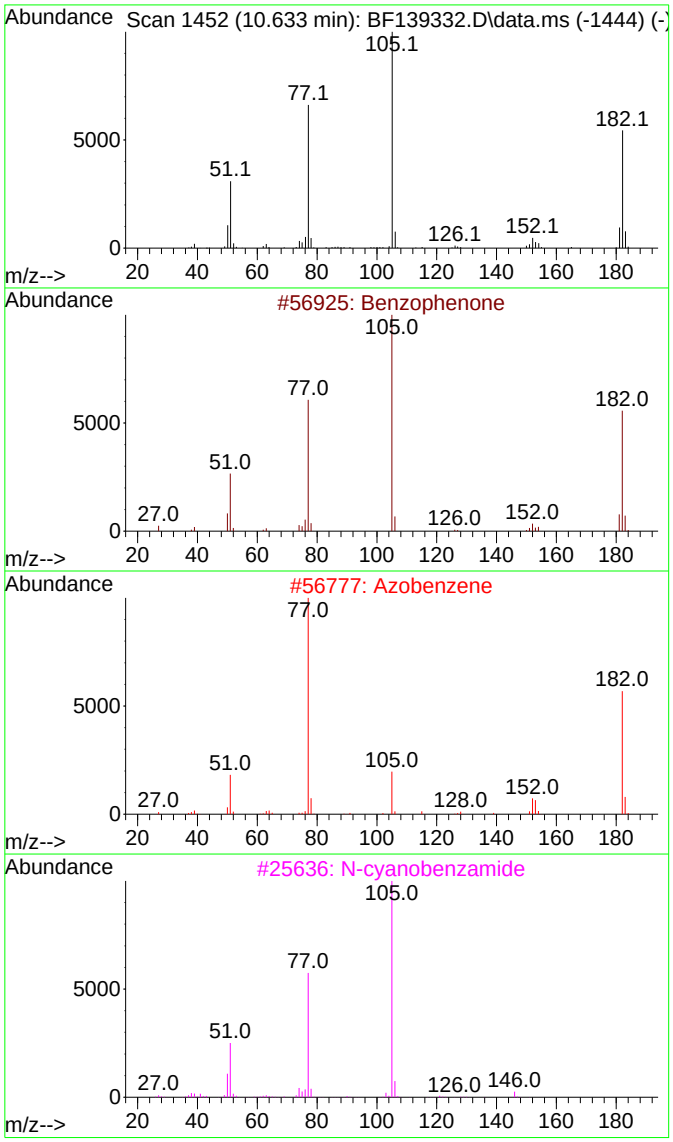
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

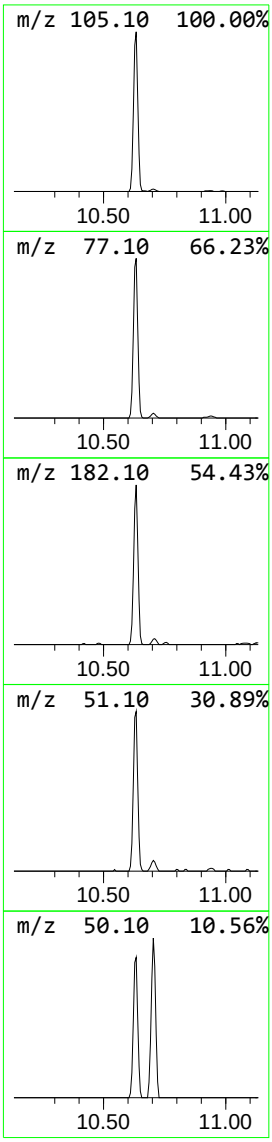
****

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.633	5.11 ng	210607	Acenaphthene-d10	9.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	52
3	N-cyanobenzamide	146	C8H6N2O	015150-25-1	47
4	5-Oxo-5-phenylpentanenitrile	173	C11H11NO	1000486-83-7	47
5	Ethanedione, diphenyl-	210	C14H10O2	000134-81-6	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139332.D
Acq On : 11 Sep 2024 18:12
Operator : RC/JU
Sample : P3929-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11930

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

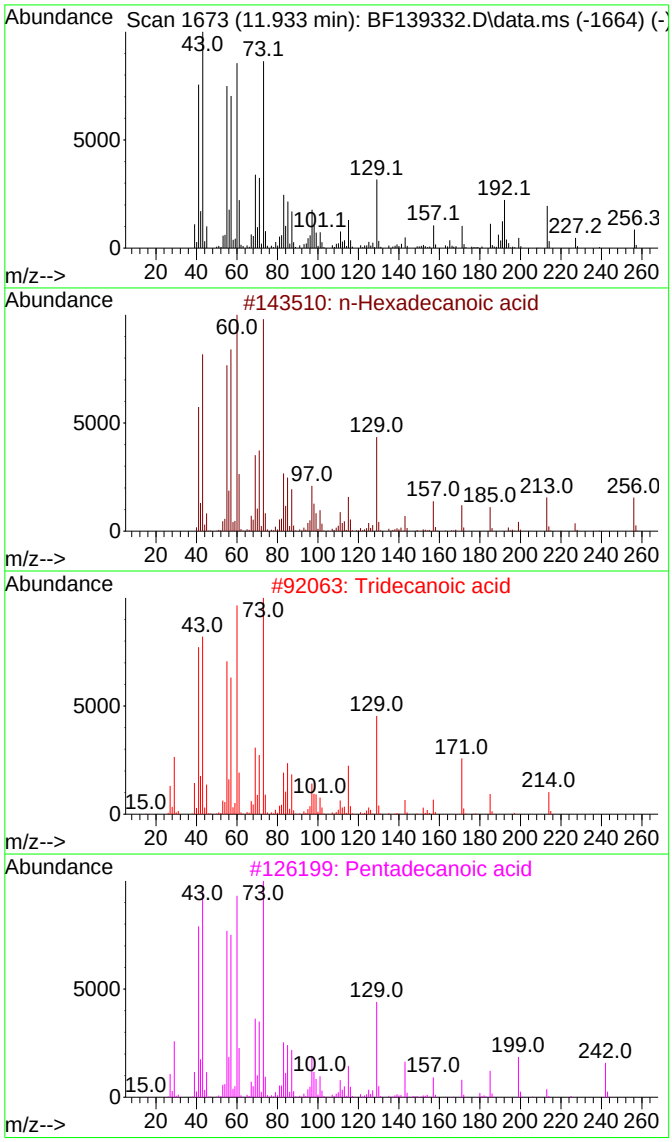
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

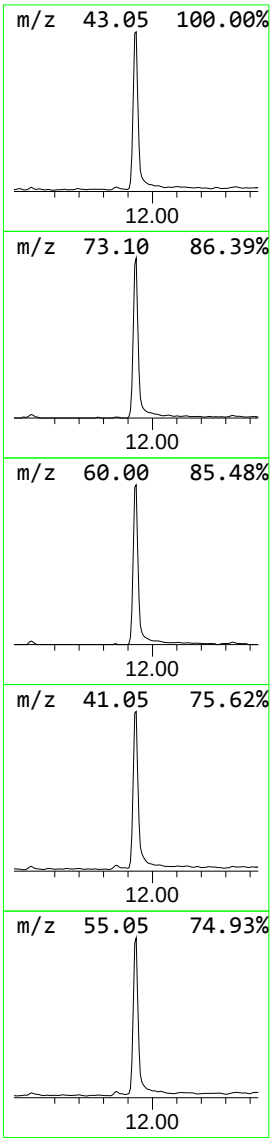
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	15.54 ng	572103	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4	n-Decanoic acid	172	C10H20O2	000334-48-5	55
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139332.D
Acq On : 11 Sep 2024 18:12
Operator : RC/JU
Sample : P3929-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11930

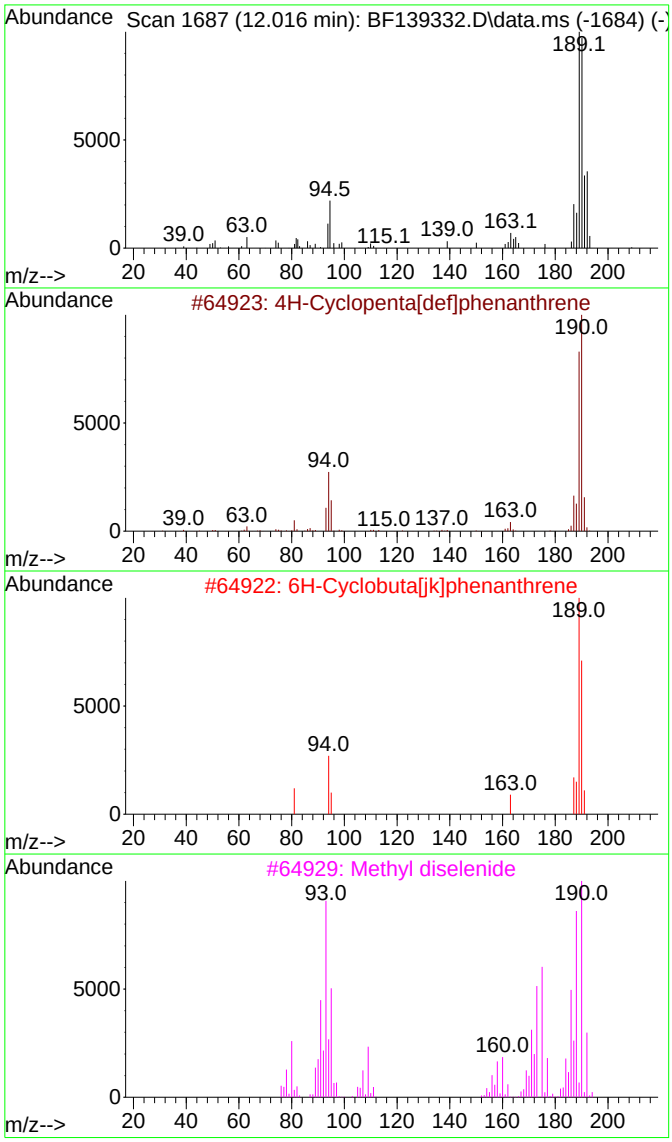
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

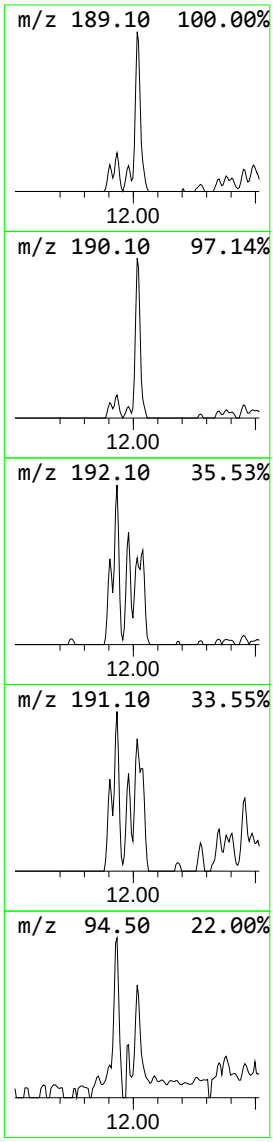
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.015	2.27 ng	83609	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	Methyl diselenide	190	C2H6Se2	007101-31-7	43
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
5	1,1'-Biphenyl, 4,4'-difluoro-	190	C12H8F2	000398-23-2	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139332.D
Acq On : 11 Sep 2024 18:12
Operator : RC/JU
Sample : P3929-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.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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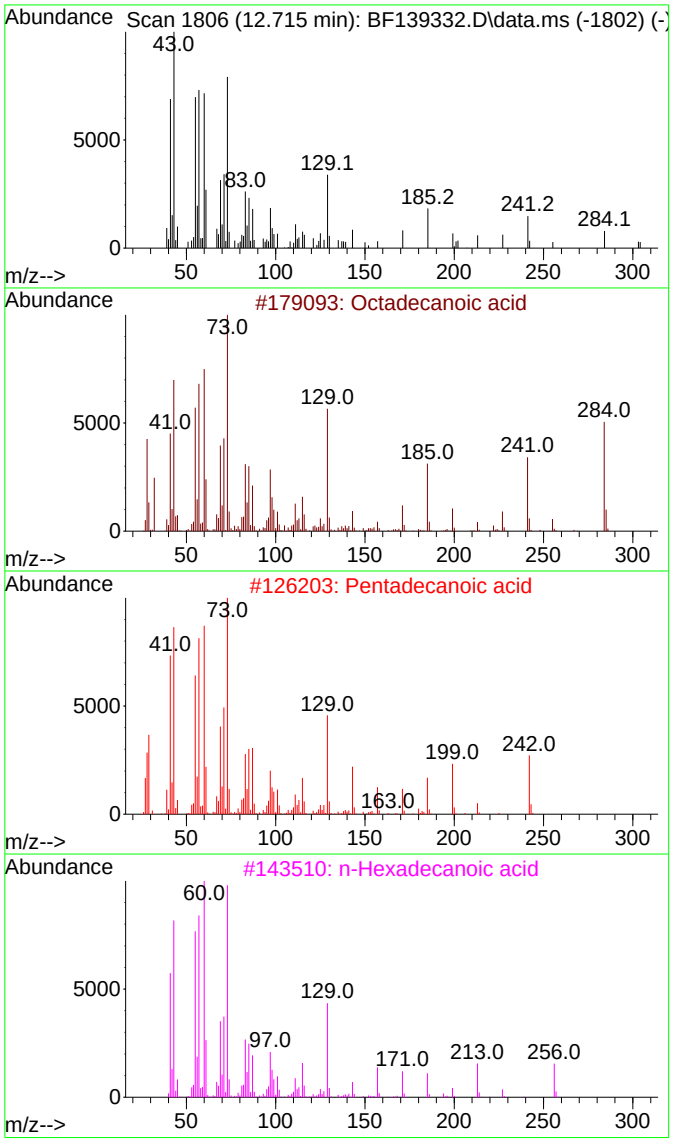
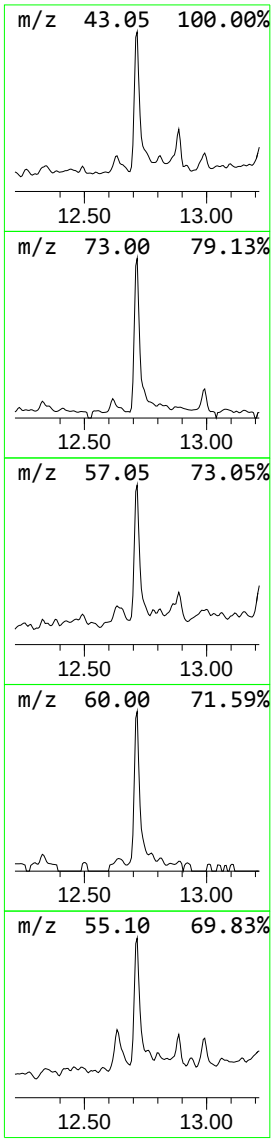
Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	2.18 ng	80169	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139332.D
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.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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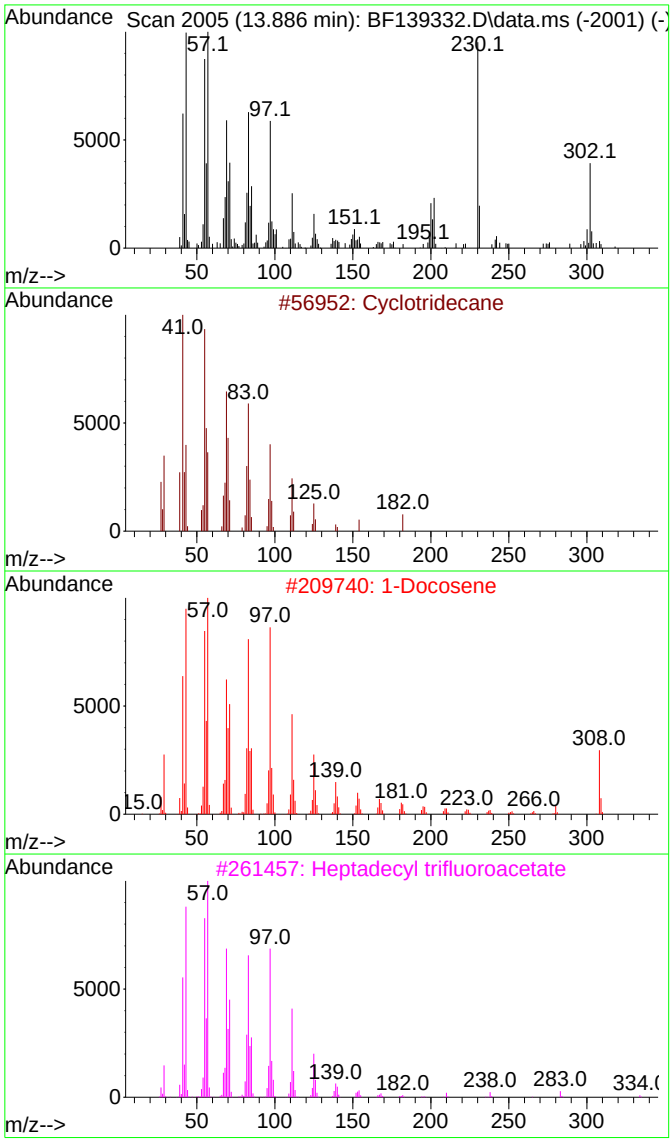
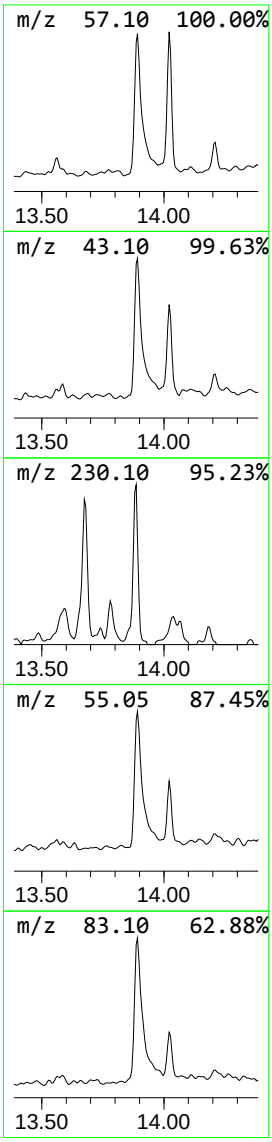
Peak Number 7 Cyclotridecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	6.17 ng	322319	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotridecane	182	C13H26	000295-02-3	62
2	1-Docosene	308	C22H44	001599-67-3	56
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	49
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	42
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139332.D
Acq On : 11 Sep 2024 18:12
Operator : RC/JU
Sample : P3929-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11930

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.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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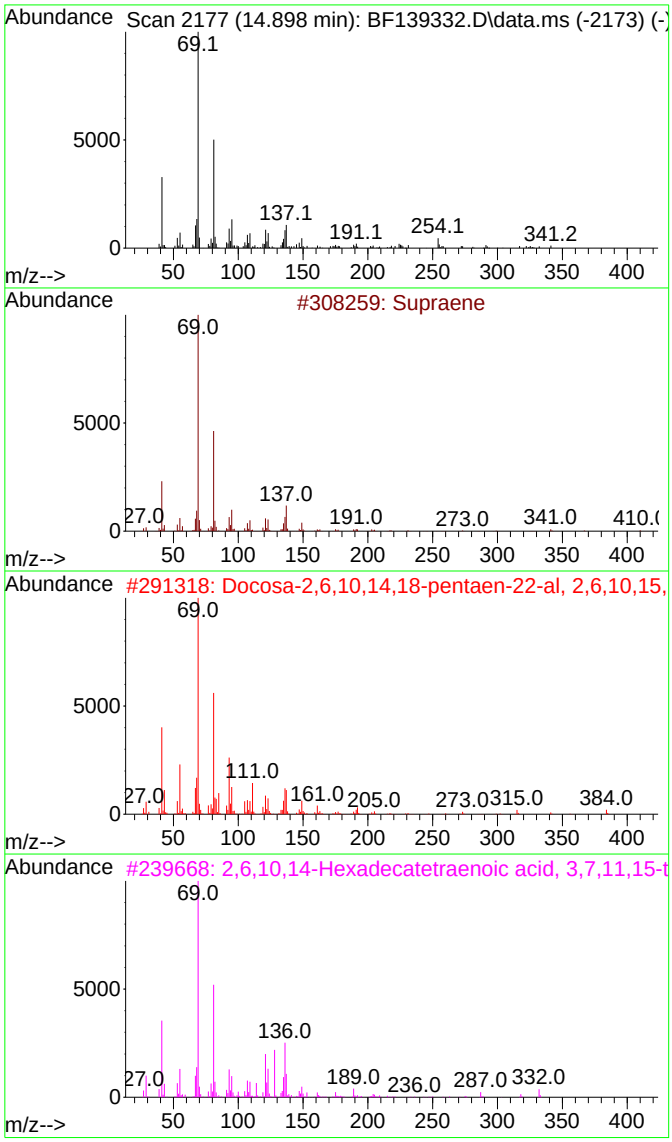
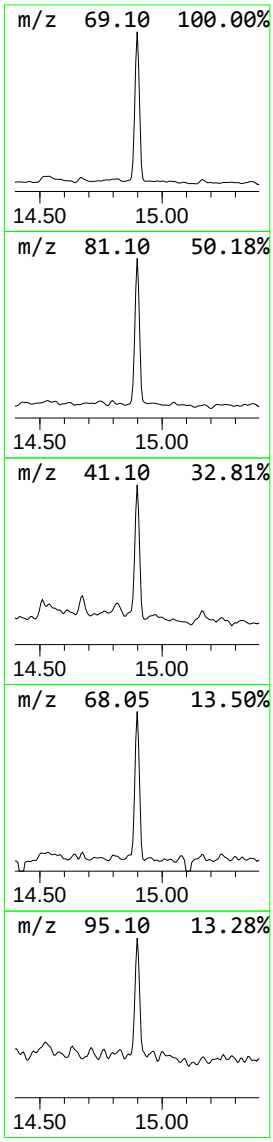
Peak Number 8 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	4.87 ng	105892	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	87
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	87
3	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	81
4	(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	64
5	Trichothec-9-en-4-ol, 7,8:12,13-...	332	C19H24O5	021284-11-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139332.D
Acq On : 11 Sep 2024 18:12
Operator : RC/JU
Sample : P3929-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11930

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

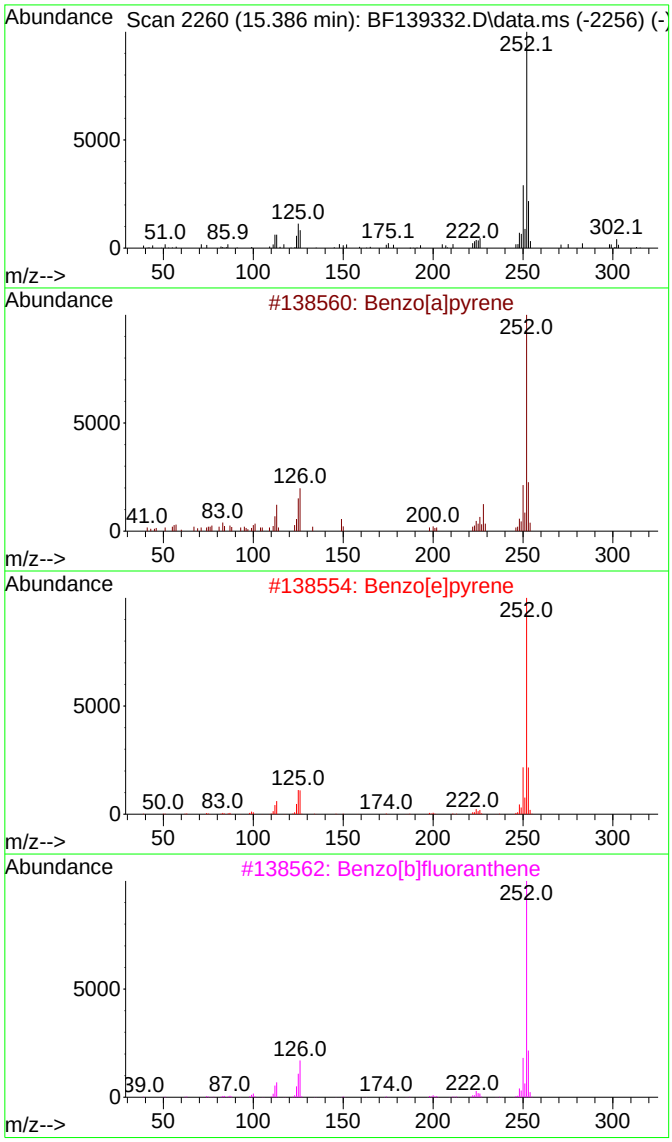
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

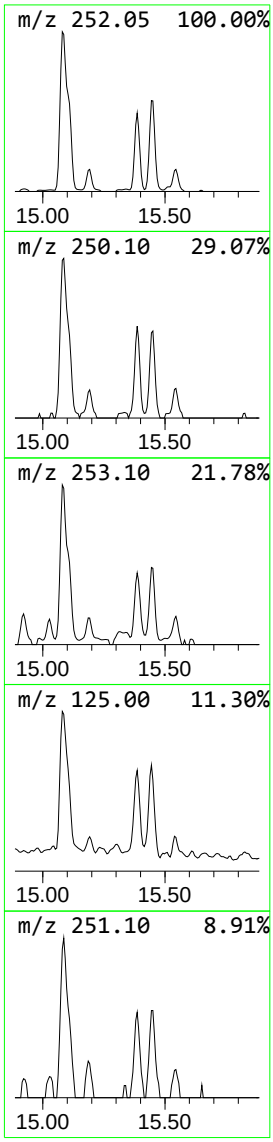
****

Peak Number 9 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.386	2.01 ng	43795	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	93
2	Benzo[e]pyrene	252	C20H12	000192-97-2	93
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
4	Perylene	252	C20H12	000198-55-0	89
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139332.D
Acq On : 11 Sep 2024 18:12
Operator : RC/JU
Sample : P3929-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11930

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.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...	2.204	105.8	ng	2145460	1	6.881	405553	20.0
2-Pentanone, 4-...	5.110	6.5	ng	131770	1	6.881	405553	20.0
Benzophenone	10.633	5.1	ng	210607	3	9.916	823609	20.0
n-Hexadecanoic ...	11.933	15.5	ng	572103	4	11.404	736351	20.0
4H-Cyclopenta[d...	12.015	2.3	ng	83609	4	11.404	736351	20.0
Octadecanoic acid	12.716	2.2	ng	80169	4	11.404	736351	20.0
Cyclotridecane	13.886	6.2	ng	322319	5	14.039	1044120	20.0
Supraene	14.898	4.9	ng	105892	6	15.515	435187	20.0
Benzo[e]pyrene	15.386	2.0	ng	43795	6	15.515	435187	20.0