LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139443.D
Acq On : 18 Sep 2024 23:35
Operator : RC/JU
Sample : P4088-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-614-COMP-09

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-BF091324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139443.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	8	16	25	rVB	738967	1145697	76.28%	8.634%
2	5.099	502	511	521	rVB	77946	118320	7.88%	0.892%
3	5.499	573	579	584	rBV	1108878	1425626	94.92%	10.744%
4	6.504	744	750	755	rBV	1126789	1501912	100.00%	11.319%
5	6.875	808	813	818	rBV	309899	390497	26.00%	2.943%
6	7.440	903	909	914	rBV	786835	996125	66.32%	7.507%
7	7.693	948	952	957	rVB	20578	25164	1.68%	0.190%
8	8.157	1024	1031	1039	rBV	369964	458438	30.52%	3.455%
9	8.375	1062	1068	1074	rBV	13122	16243	1.08%	0.122%
10	9.234	1208	1214	1219	rBV	1218291	1492255	99.36%	11.246%
11	9.910	1324	1329	1334	rBV	333927	402448	26.80%	3.033%
12	10.622	1445	1450	1457	rBV	223325	269985	17.98%	2.035%
13	10.698	1457	1463	1473	rVV	551301	693421	46.17%	5.226%
14	10.816	1479	1483	1491	rVB4	8901	15051	1.00%	0.113%
15	10.933	1498	1503	1509	rVB	37757	48690	3.24%	0.367%
16	11.392	1576	1581	1590	rBV2	279537	446659	29.74%	3.366%
17	11.469	1590	1594	1598	rVB	15920	19230	1.28%	0.145%
18	11.916	1663	1670	1676	rBV2	84619	146711	9.77%	1.106%
19	12.010	1682	1686	1694	rVB	27503	52109	3.47%	0.393%
20	12.192	1712	1717	1719	rBV	12930	19547	1.30%	0.147%
21	12.480	1763	1766	1771	rVB4	10776	15307	1.02%	0.115%
22	12.527	1771	1774	1779	rVB	13265	15669	1.04%	0.118%
23	12.604	1783	1787	1792	rBV	213864	276103	18.38%	2.081%
24	12.704	1800	1804	1807	rBV	16709	23026	1.53%	0.174%
25	12.833	1819	1826	1832	rVV	187344	280297	18.66%	2.112%
26	12.980	1844	1851	1857	rVB	829222	1084163	72.19%	8.170%
27	13.051	1858	1863	1871	rBV3	20631	40160	2.67%	0.303%
28	13.163	1875	1882	1885	rVB2	27557	48846	3.25%	0.368%
29	13.227	1891	1893	1896	rVV	17085	19264	1.28%	0.145%
30	13.263	1896	1899	1907	rVB3	23208	38003	2.53%	0.286%
31	13.551	1944	1948	1961	rVB5	16532	38482	2.56%	0.290%
32	13.669	1964	1968	1976	rVB	20850	31512	2.10%	0.237%
33	13.780	1982	1987	1989	rBV2	24582	37919	2.52%	0.286%
34	13.874	1999	2003	2012	rVB	80529	124191	8.27%	0.936%
35	14.027	2022	2029	2041	rBV2	310523	647980	43.14%	4.883%
36	14.504	2106	2110	2114	rBV3	27447	51023	3.40%	0.385%

LSC Area Percent Report

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Instrument :
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ClientSampleId :
NB-614-COMP-09

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-BF091324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.074	2201	2207	2215	rBV	91572	204998	13.65%	1.545%
38	15.180	2222	2225	2229	rVB	15254	18033	1.20%	0.136%
39	15.374	2254	2258	2263	rVB	46250	71449	4.76%	0.538%
40	15.433	2264	2268	2274	rVV	60869	102144	6.80%	0.770%
41	15.498	2274	2279	2291	rVB2	142649	276613	18.42%	2.085%
42	16.210	2397	2400	2409	rVB7	17335	33482	2.23%	0.252%
43	16.962	2524	2528	2536	rVB2	28268	58970	3.93%	0.444%
44	17.410	2599	2604	2617	rVB	20318	47493	3.16%	0.358%

Sum of corrected areas: 13269255

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Instrument :
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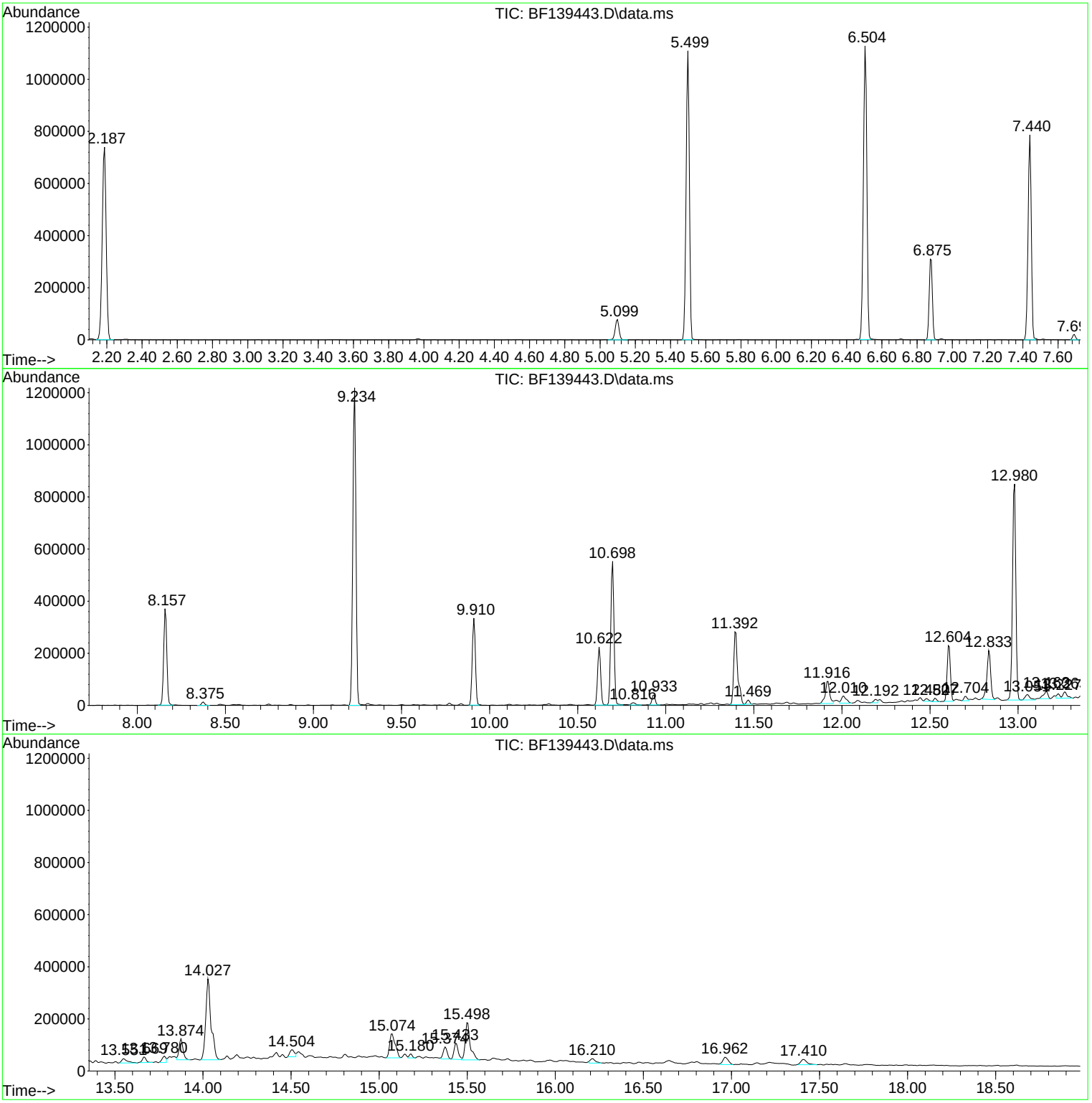
ClientSampleId :
NB-614-COMP-09

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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\BF091824\
Data File : BF139443.D
Acq On : 18 Sep 2024 23:35
Operator : RC/JU
Sample : P4088-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-614-COMP-09

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

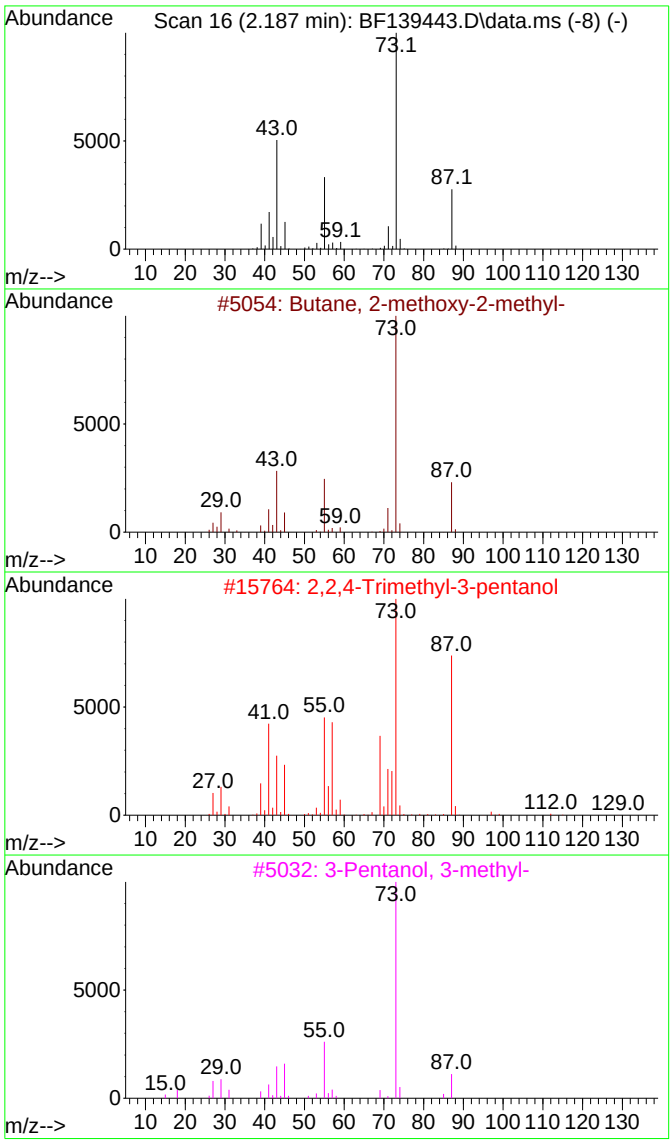
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

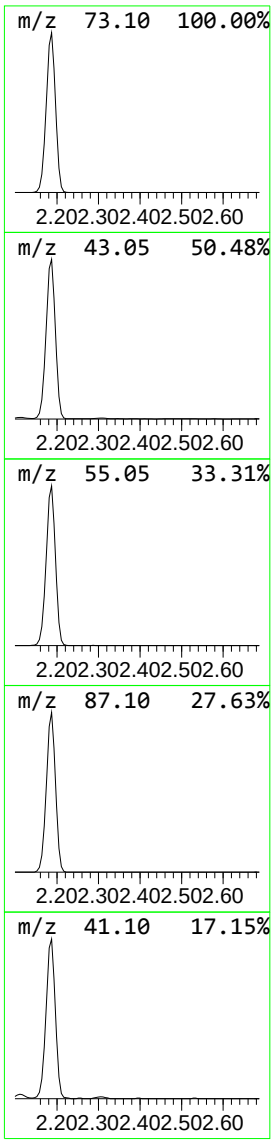
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	58.68 ng	1145700	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	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Sample : P4088-13
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ALS Vial : 17 Sample Multiplier: 1

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ClientSampleId :
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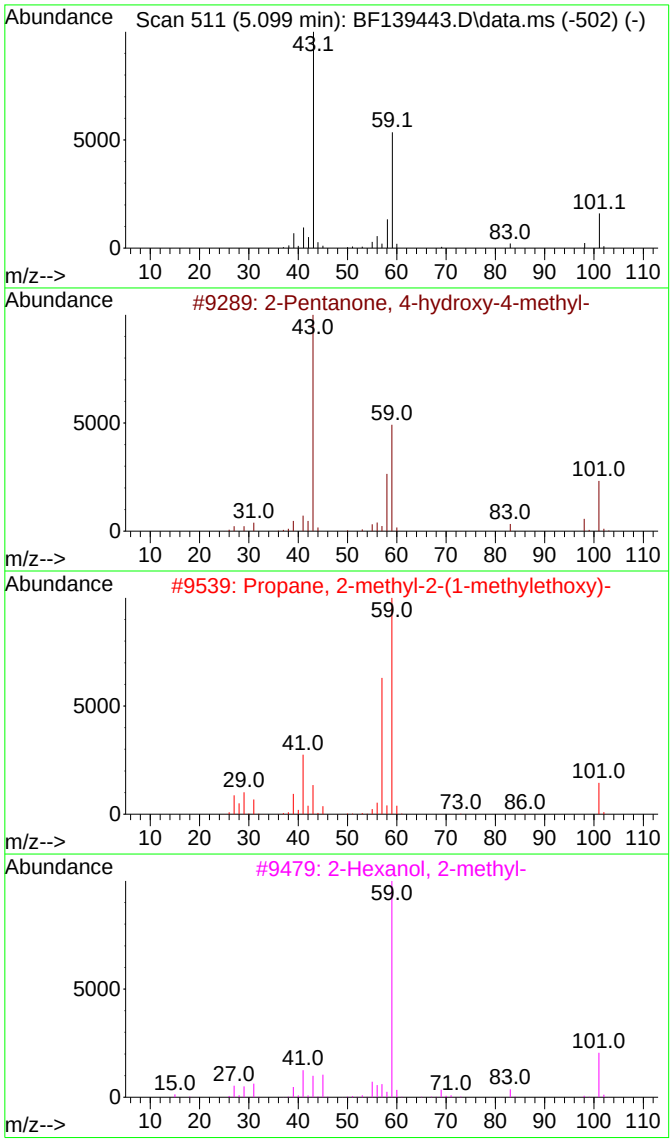
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

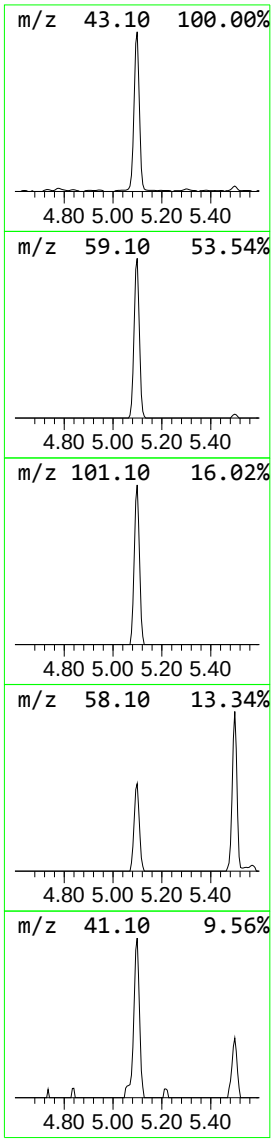
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.099	6.06 ng	118320	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	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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Operator : RC/JU
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Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

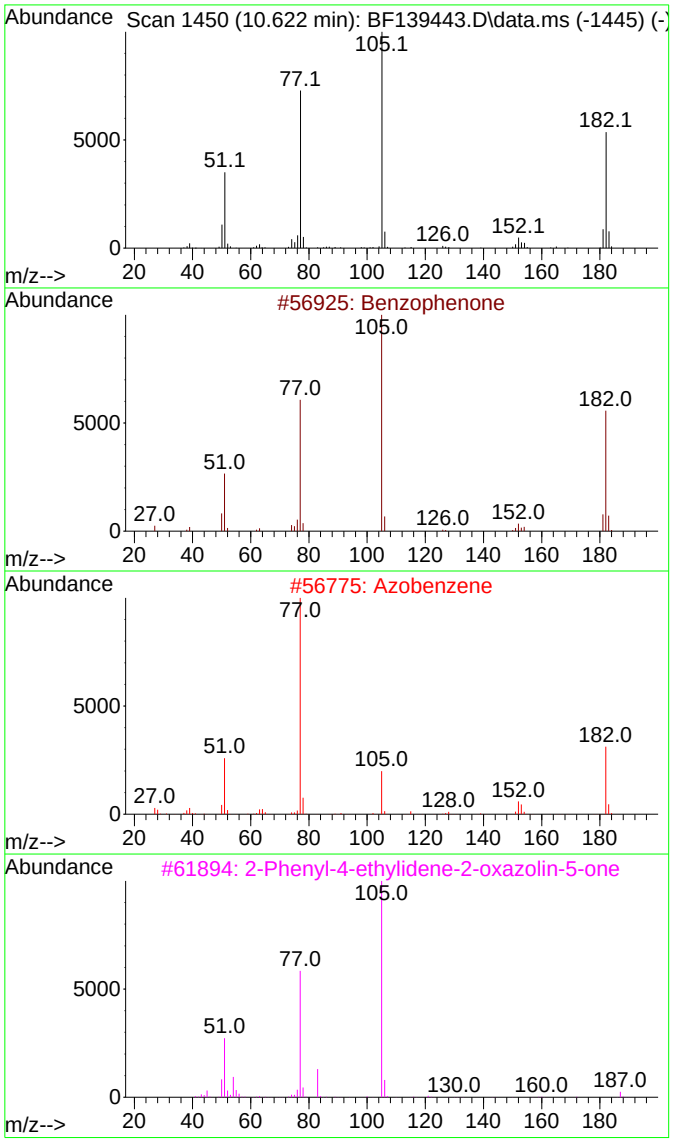
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

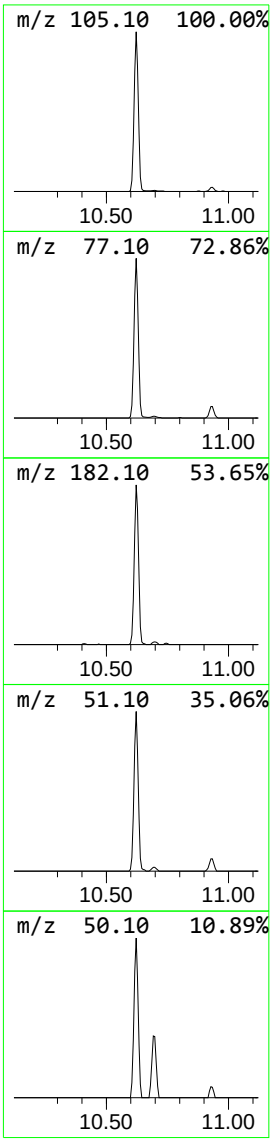
****

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	13.42 ng	269985	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	64
3	2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	50
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
5	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50





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Sample : P4088-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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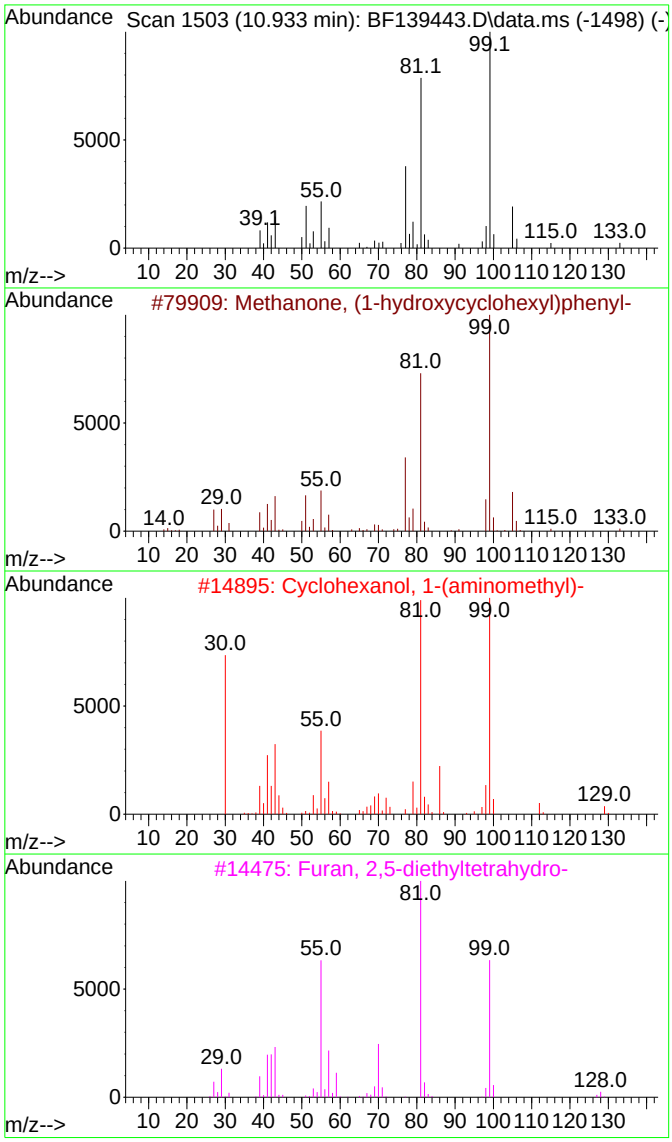
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

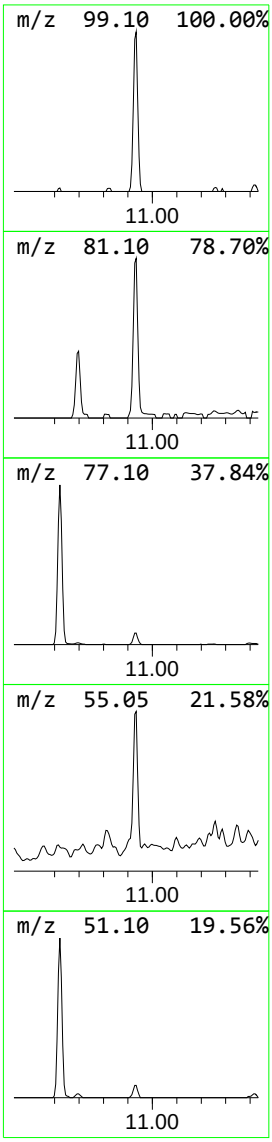
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Methanone, (1-hydroxycycloh... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.934	2.18 ng	48690	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	90
2	Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	59
3	Furan, 2,5-diethyltetrahydro-	128	C8H16O	041239-48-9	42
4	3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	40
5	1-(Prop-2-yn-1-yl)cyclohexyl car...	181	C10H15NO2	000358-52-1	36





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Sample : P4088-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-614-COMP-09

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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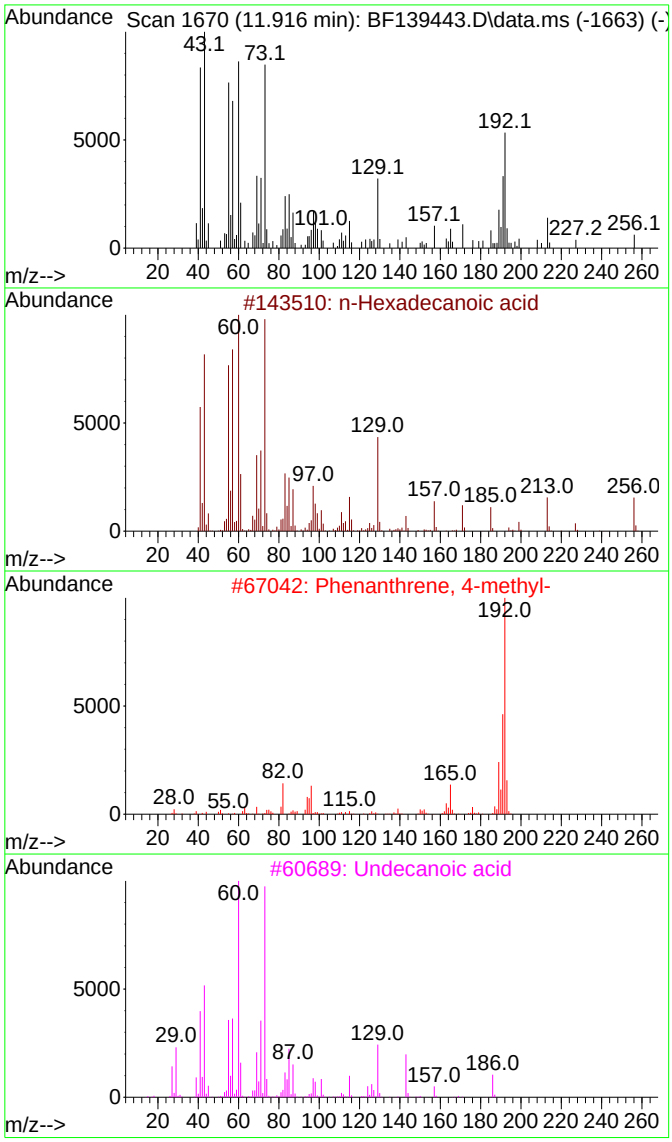
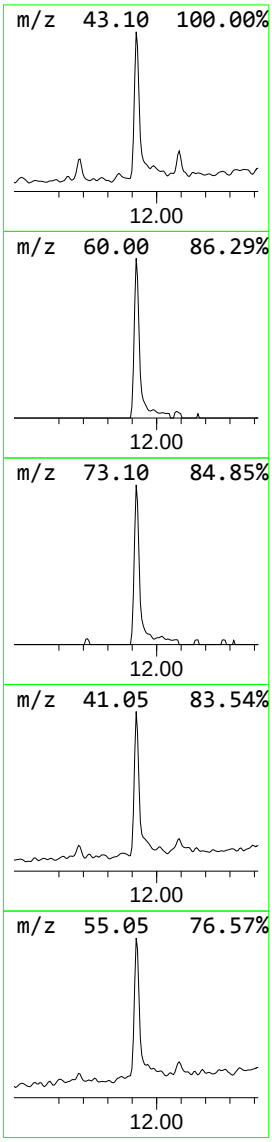
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	6.57 ng	146711	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	90
3	Undecanoic acid	186	C11H22O2	000112-37-8	60
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	60
5	Tridecanoic acid	214	C13H26O2	000638-53-9	55





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

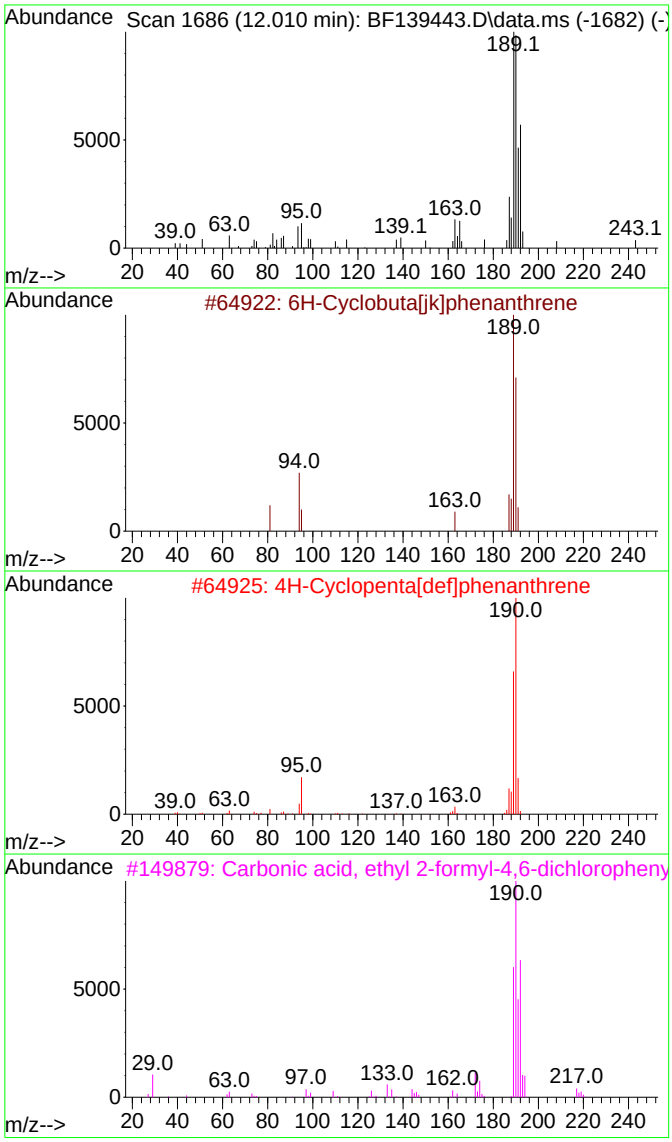
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

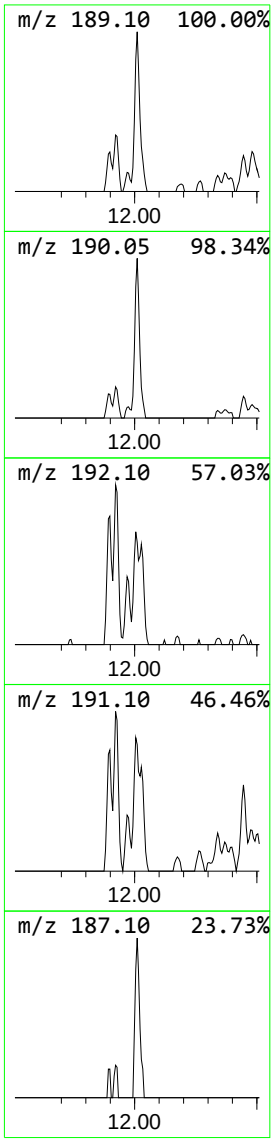
****

Peak Number 6 6H-Cyclobuta[jk]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	2.33 ng	52109	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	58
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	53
3	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	40
4	2-Amino-4,6-dichloropyrimidine-5...	191	C5H3Cl2N3O	005604-46-6	38
5	4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	37





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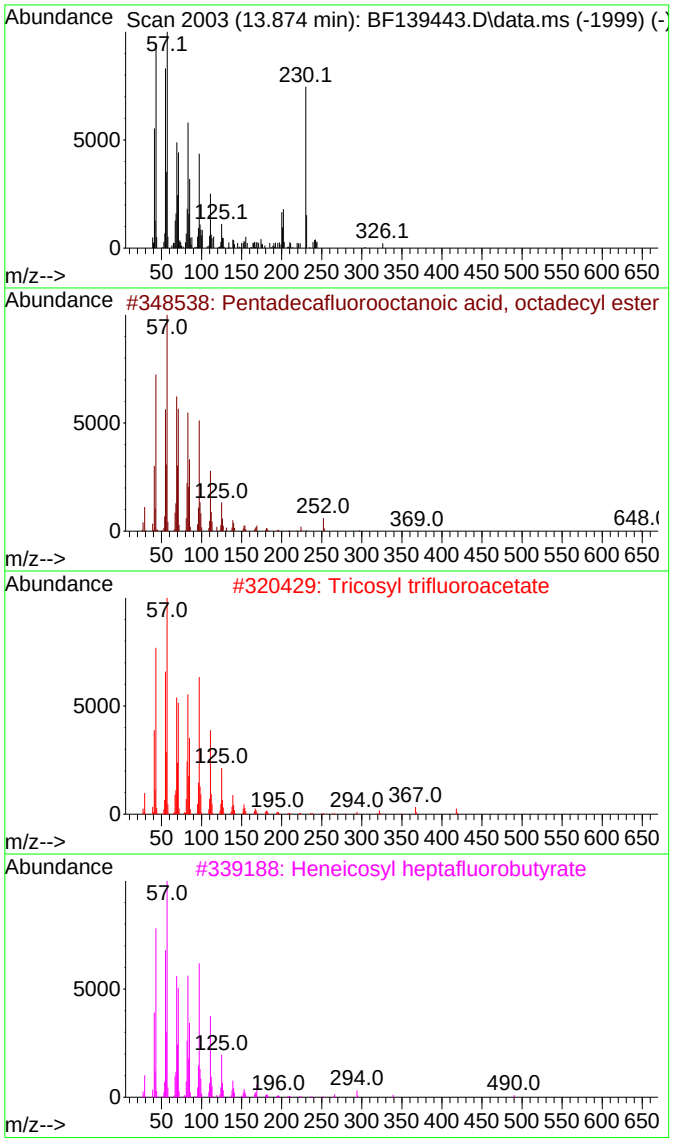
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

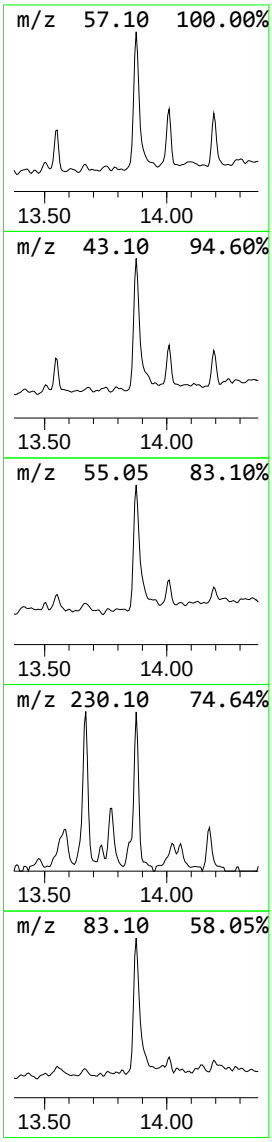
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	3.83 ng	124191	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87
2	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	55
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	55
4	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	55
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	55





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Data File : BF139443.D
Acq On : 18 Sep 2024 23:35
Operator : RC/JU
Sample : P4088-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-614-COMP-09

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

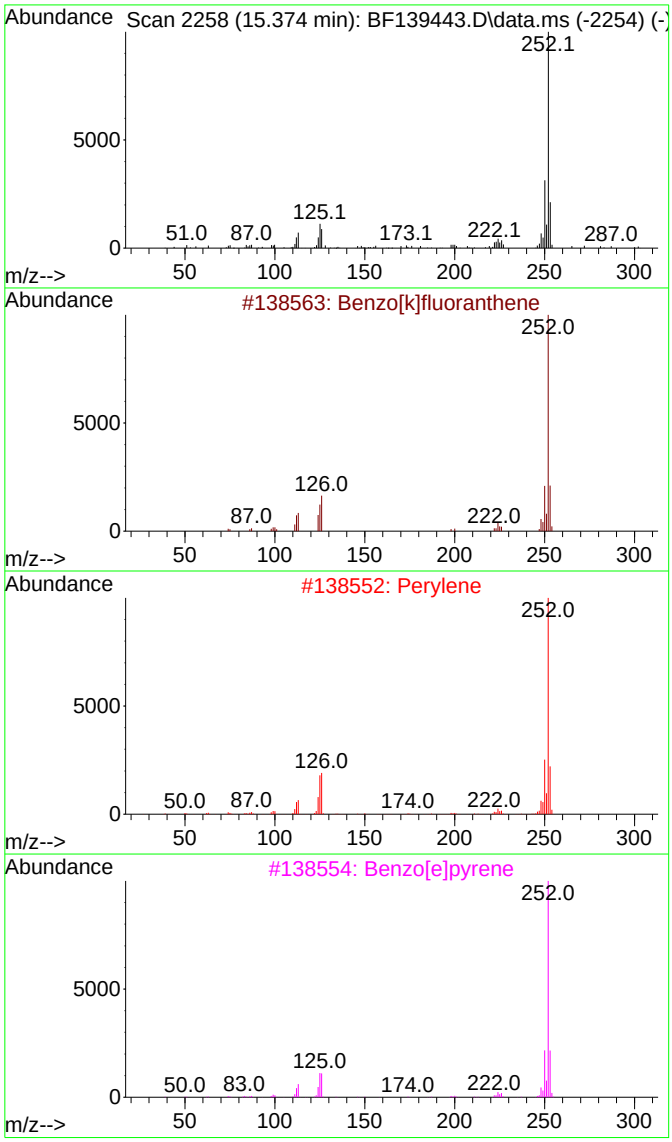
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

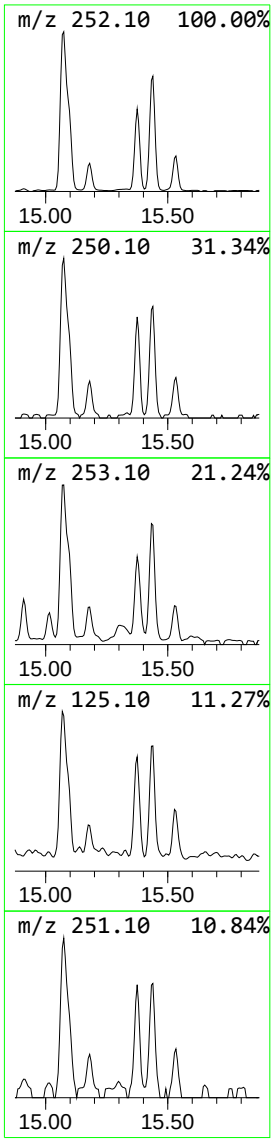
****

Peak Number 8 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.374	5.17 ng	71449	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
2	Perylene	252	C20H12	000198-55-0	94
3	Benzo[e]pyrene	252	C20H12	000192-97-2	94
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139443.D
Acq On : 18 Sep 2024 23:35
Operator : RC/JU
Sample : P4088-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-614-COMP-09

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

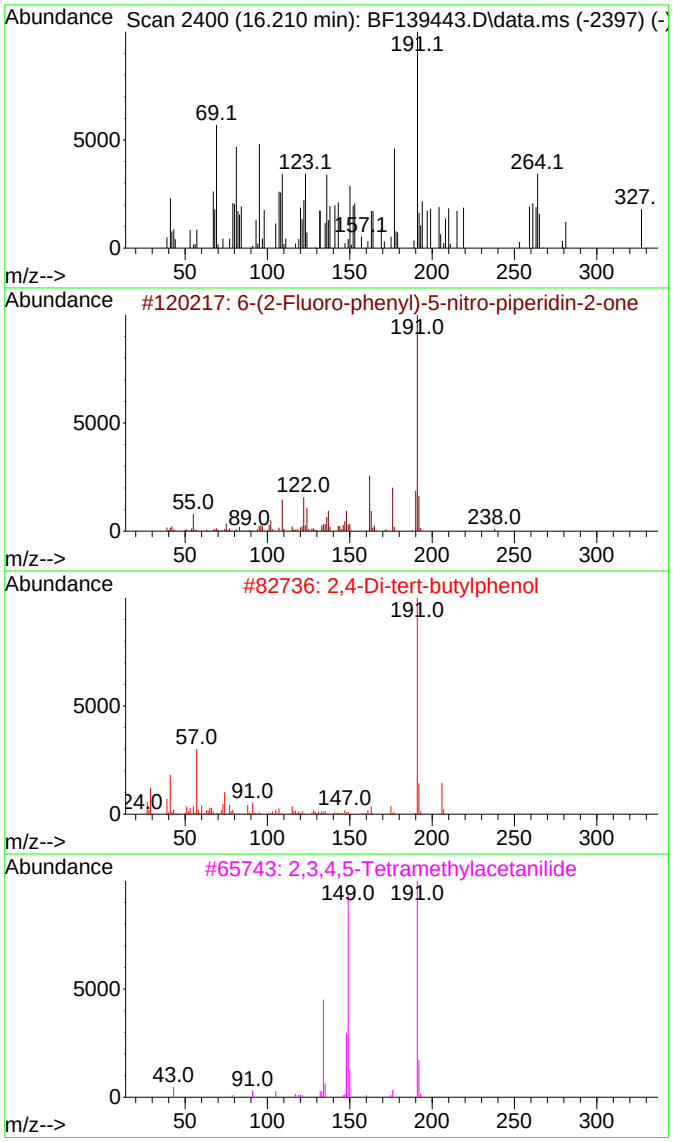
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

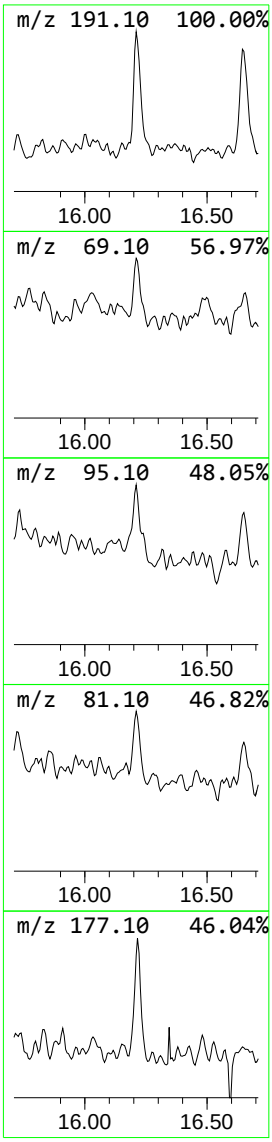
****

Peak Number 9 unknown16.210 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.210	2.42 ng	33482	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-(2-Fluoro-phenyl)-5-nitro-pipe...	238	C11H11FN2O3	1000275-16-4	14
2	2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	14
3	2,3,4,5-Tetramethylacetanilide	191	C12H17NO	1000432-93-7	14
4	2-(2,4-Difluorophenyl)pyridine	191	C11H7F2N	391604-55-0	14
5	Carbonic acid, monoamide, N-meth...	191	C11H13NO2	1000340-18-1	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091824\
Data File : BF139443.D
Acq On : 18 Sep 2024 23:35
Operator : RC/JU
Sample : P4088-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-614-COMP-09

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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...	2.187	58.7	ng	1145700	1	6.881	390497	20.0
2-Pentanone, 4-...	5.099	6.1	ng	118320	1	6.881	390497	20.0
Benzophenone	10.622	13.4	ng	269985	3	9.910	402448	20.0
Methanone, (1-h...	10.934	2.2	ng	48690	4	11.392	446659	20.0
n-Hexadecanoic ...	11.916	6.6	ng	146711	4	11.392	446659	20.0
6H-Cyclobuta[jk...	12.010	2.3	ng	52109	4	11.392	446659	20.0
Pentadecafluoro...	13.874	3.8	ng	124191	5	14.033	647980	20.0
Perylene	15.374	5.2	ng	71449	6	15.504	276613	20.0
unknown16.210	16.210	2.4	ng	33482	6	15.504	276613	20.0