LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136435.D
Acq On : 06 Dec 2023 18:48
Operator : CG\JU
Sample : 05463-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-11162023

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-BF120523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136435.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	15	20	26	rBV	22888	32634	1.65%	0.200%
2	5.034	496	501	506	rBV	123648	148242	7.50%	0.908%
3	5.434	564	569	572	rBV	2095885	1857333	93.97%	11.380%
4	6.434	734	739	742	rBV	1895444	1706162	86.32%	10.453%
5	6.634	770	773	785	rBV2	16964	40040	2.03%	0.245%
6	6.798	797	801	804	rBV	559826	452619	22.90%	2.773%
7	7.357	891	896	899	rBV	1232611	1024436	51.83%	6.277%
8	8.075	1012	1018	1021	rBV	614510	518499	26.23%	3.177%
9	8.498	1086	1090	1092	rBV	30679	32723	1.66%	0.200%
10	9.098	1189	1192	1197	rBV2	54016	51469	2.60%	0.315%
11	9.151	1197	1201	1204	rBV	2204999	1723417	87.19%	10.559%
12	9.233	1212	1215	1218	rBV2	24631	25965	1.31%	0.159%
13	9.275	1218	1222	1232	rVB	467744	484723	24.52%	2.970%
14	9.557	1264	1270	1272	rVB2	35253	41112	2.08%	0.252%
15	9.692	1290	1293	1298	rVB	23216	24067	1.22%	0.147%
16	9.828	1310	1316	1320	rBV	576030	495646	25.08%	3.037%
17	9.863	1320	1322	1326	rVB2	24232	22711	1.15%	0.139%
18	10.375	1407	1409	1412	rBV	25870	25881	1.31%	0.159%
19	10.622	1447	1451	1454	rBV	1214827	1011603	51.18%	6.198%
20	10.745	1469	1472	1479	rVB3	21429	32992	1.67%	0.202%
21	11.216	1550	1552	1557	rVB2	22147	23547	1.19%	0.144%
22	11.322	1566	1570	1572	rBV	644468	532881	26.96%	3.265%
23	11.345	1572	1574	1578	rVV	258028	201120	10.18%	1.232%
24	11.392	1578	1582	1586	rVB	64178	64643	3.27%	0.396%
25	11.722	1635	1638	1644	rVB4	17523	28673	1.45%	0.176%
26	11.827	1652	1656	1658	rBV	38987	40663	2.06%	0.249%
27	11.857	1658	1661	1665	rVV2	213877	195124	9.87%	1.195%
28	11.933	1671	1674	1677	rBV	78115	82002	4.15%	0.502%
29	11.957	1677	1678	1684	rVB	34763	27852	1.41%	0.171%
30	12.116	1701	1705	1708	rBV2	35898	51616	2.61%	0.316%
31	12.145	1708	1710	1715	rVB3	35244	37130	1.88%	0.227%
32	12.374	1746	1749	1752	rBV	38147	41436	2.10%	0.254%
33	12.416	1752	1756	1757	rVV3	39328	44683	2.26%	0.274%
34	12.433	1757	1759	1761	rVV2	78238	60219	3.05%	0.369%
35	12.463	1761	1764	1768	rVB4	26830	32538	1.65%	0.199%
36	12.539	1773	1777	1780	rBV	576993	452937	22.91%	2.775%

LSC Area Percent Report

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Data File : BF136435.D
Acq On : 06 Dec 2023 18:48
Operator : CG\JU
Sample : 05463-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-11162023

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-BF120523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.580	1781	1784	1787	rVV3	19054	24890	1.26%	0.152%
38	12.645	1791	1795	1801	rBV5	64486	95262	4.82%	0.584%
39	12.769	1810	1816	1819	rBV	463527	466844	23.62%	2.860%
40	12.816	1823	1824	1830	rVB3	16750	21729	1.10%	0.133%
41	12.886	1833	1836	1837	rBV3	26731	23116	1.17%	0.142%
42	12.916	1837	1841	1845	rVB	2115950	1976608	100.00%	12.110%
43	12.986	1850	1853	1857	rVV2	29469	41197	2.08%	0.252%
44	13.074	1866	1868	1870	rBV3	26808	30037	1.52%	0.184%
45	13.098	1870	1872	1876	rVB	72149	62078	3.14%	0.380%
46	13.163	1879	1883	1886	rBV2	54877	70676	3.58%	0.433%
47	13.204	1886	1890	1893	rBV2	47192	56676	2.87%	0.347%
48	13.292	1903	1905	1908	rVB	26248	22570	1.14%	0.138%
49	13.327	1908	1911	1913	rBV	28227	24883	1.26%	0.152%
50	13.498	1938	1940	1943	rBV4	27178	26524	1.34%	0.163%
51	13.610	1957	1959	1963	rVB	37410	39524	2.00%	0.242%
52	13.721	1976	1978	1980	rVB	37641	27936	1.41%	0.171%
53	13.751	1981	1983	1985	rBV	27576	21900	1.11%	0.134%
54	13.821	1992	1995	1999	rVB2	31929	43124	2.18%	0.264%
55	13.974	2016	2021	2023	rBV2	496794	608963	30.81%	3.731%
56	13.998	2023	2025	2028	rVB	173532	126986	6.42%	0.778%
57	14.457	2100	2103	2106	rVB3	55072	54350	2.75%	0.333%
58	15.015	2195	2198	2202	rBV	137099	213866	10.82%	1.310%
59	15.321	2248	2250	2257	rVB	85741	118237	5.98%	0.724%
60	15.386	2258	2261	2268	rVB	111267	141876	7.18%	0.869%
61	15.457	2268	2273	2276	rBV	242341	312388	15.80%	1.914%

Sum of corrected areas: 16321578

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Instrument :
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ClientSampleId :
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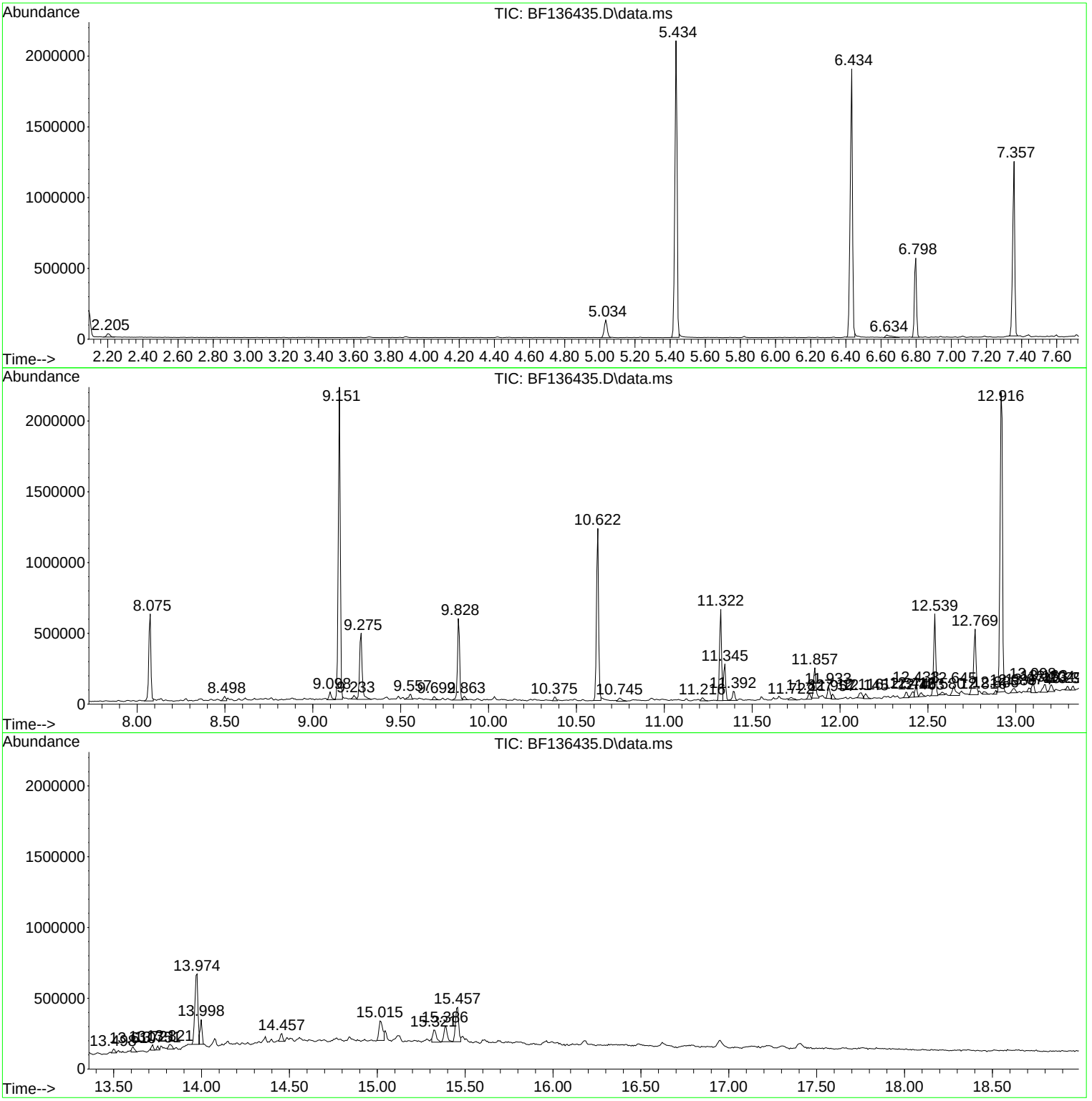
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF136435.D
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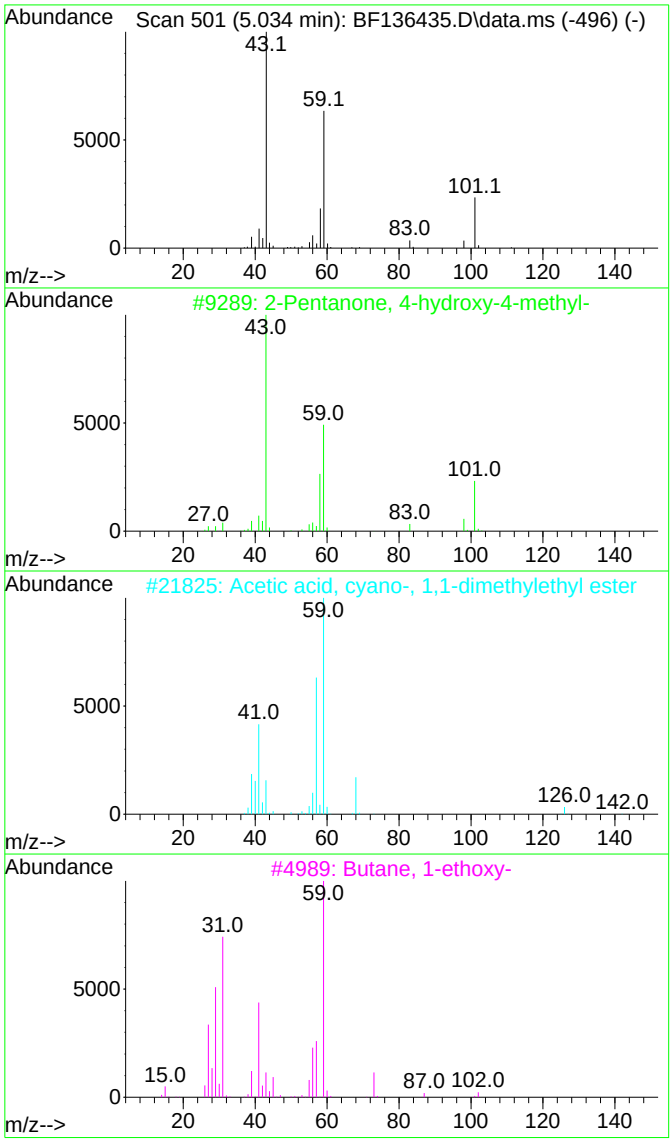
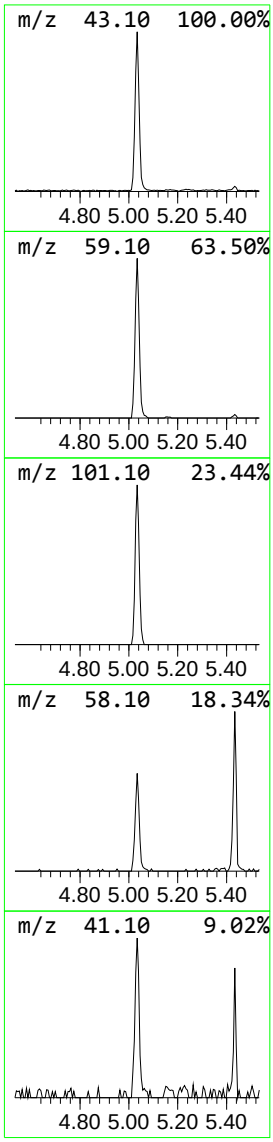
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	6.55 ng	148242	1,4-Dichlorobenzene-d4	6.798

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	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Guanidine	59	CH5N3	000113-00-8	9





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Operator : CG\JU
Sample : 05463-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-11162023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

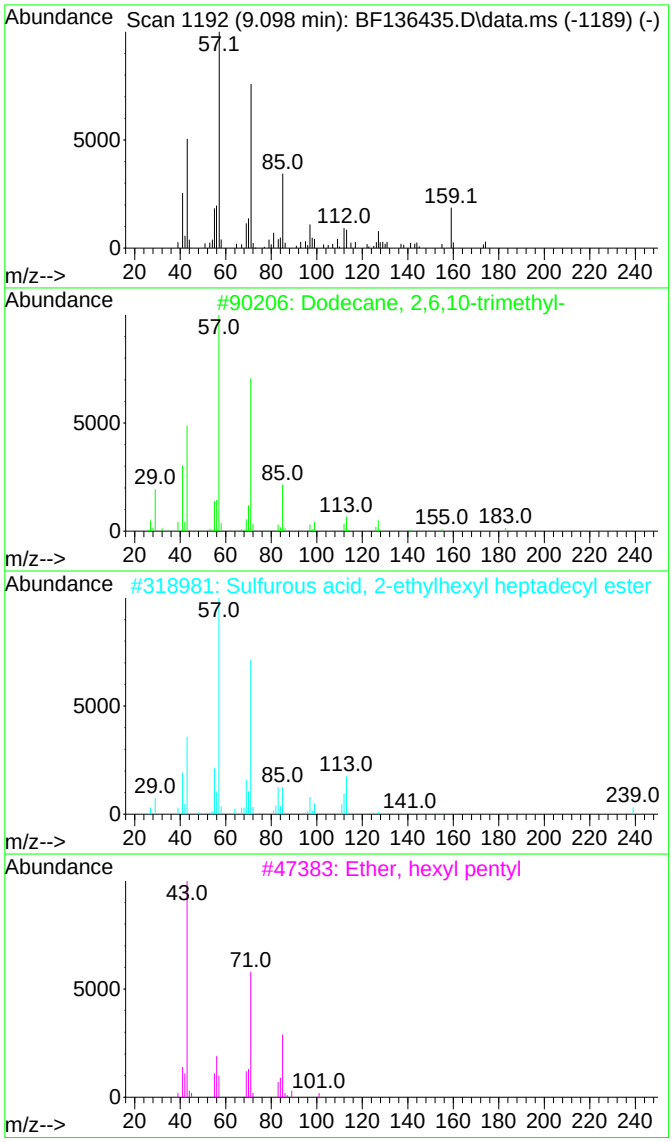
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

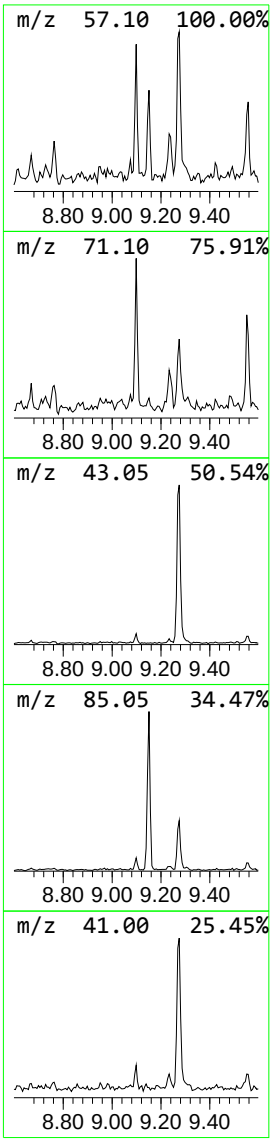
****

Peak Number 2 Dodecane, 2,6,10-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.098	2.08 ng	51469	Acenaphthene-d10	9.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	64
2	Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	53
3	Ether, hexyl pentyl	172	C11H24O	032357-83-8	47
4	2-Decanol, 2-methylpropionate	228	C14H28O2	1000447-30-4	47
5	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-11162023

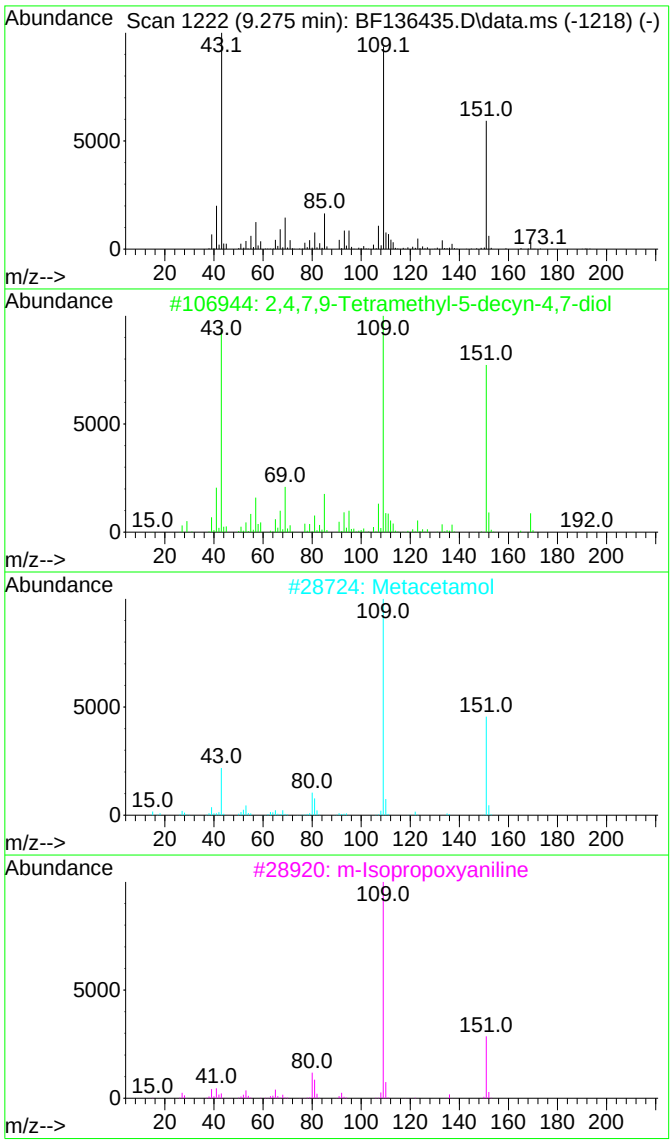
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

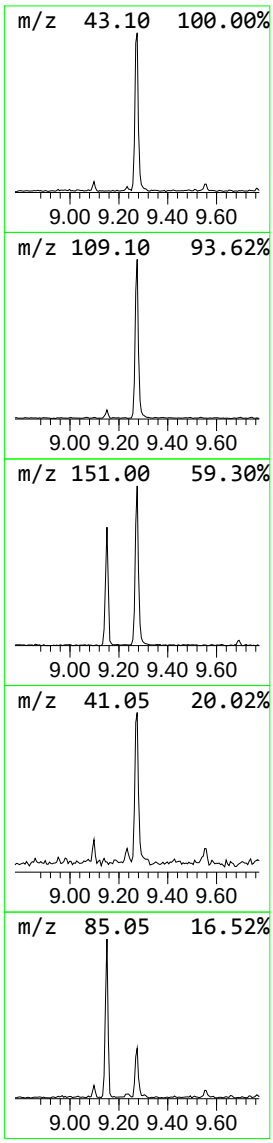
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.275	19.56 ng	484723	Acenaphthene-d10	9.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Metacetamol	151	C8H9NO2	000621-42-1	59
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	59
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	45
5	3,3,5,5-Tetramethylcyclopentene	124	C9H16	038667-10-6	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

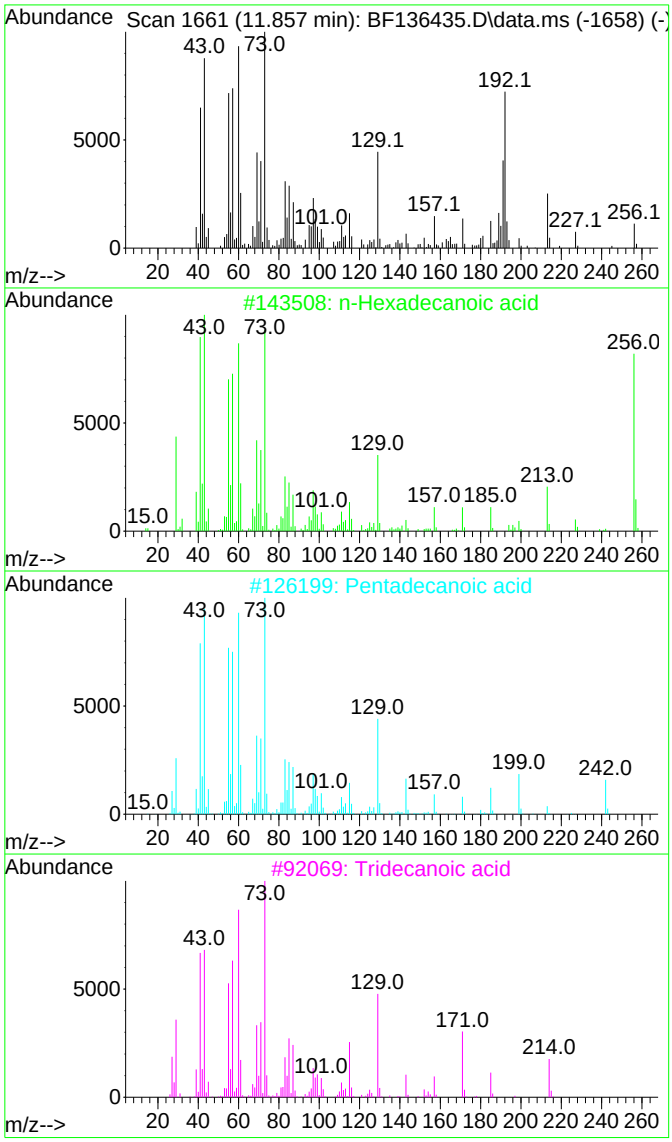
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

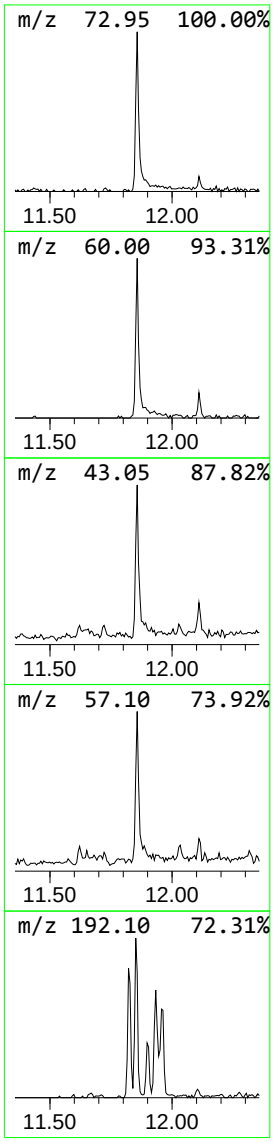
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	7.32 ng	195124	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	60





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Sample : 05463-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-11162023

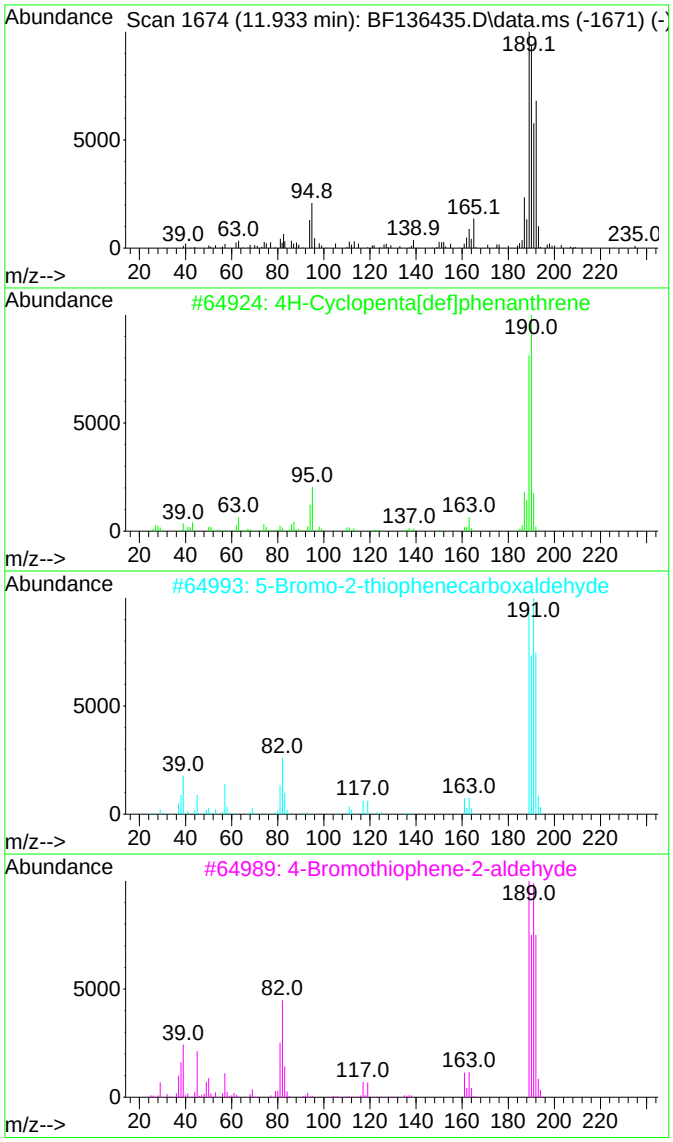
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

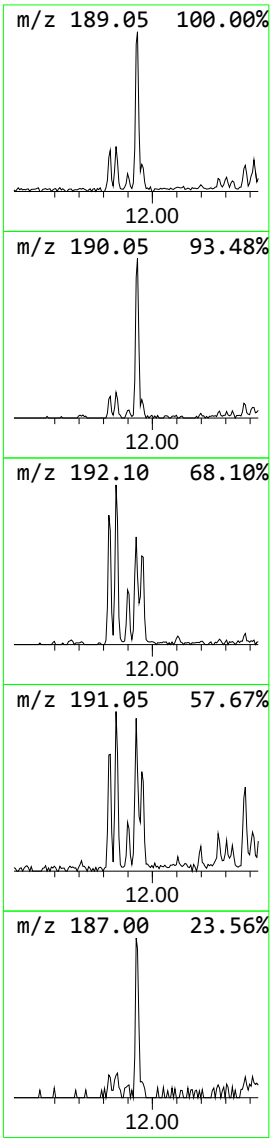
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	3.08 ng	82002	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	52
3	4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	50
4	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	50
5	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	38





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BNA_F
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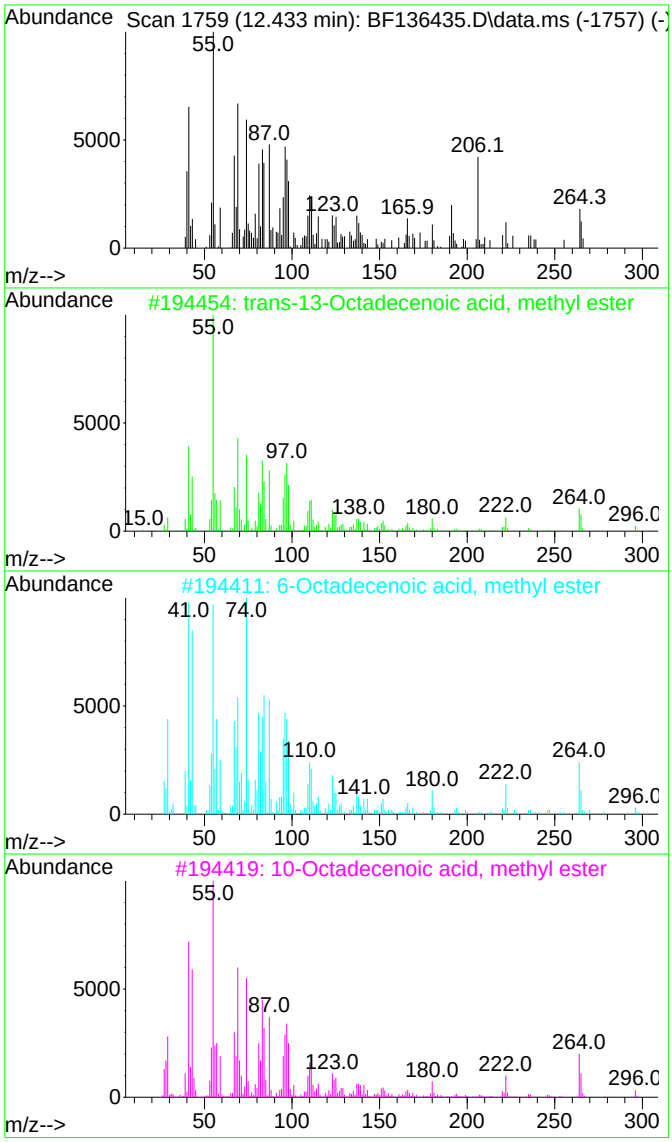
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

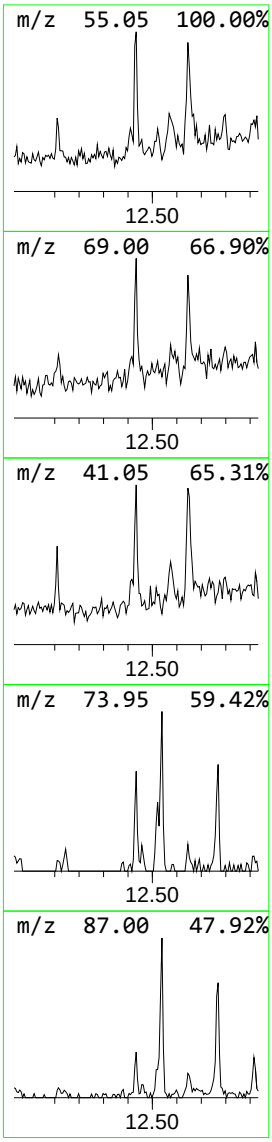
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 trans-13-Octadecenoic acid,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.433	2.26 ng	60219	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	76
2	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	76
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	76
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	76
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	70





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Data File : BF136435.D
Acq On : 06 Dec 2023 18:48
Operator : CG\JU
Sample : 05463-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-11162023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

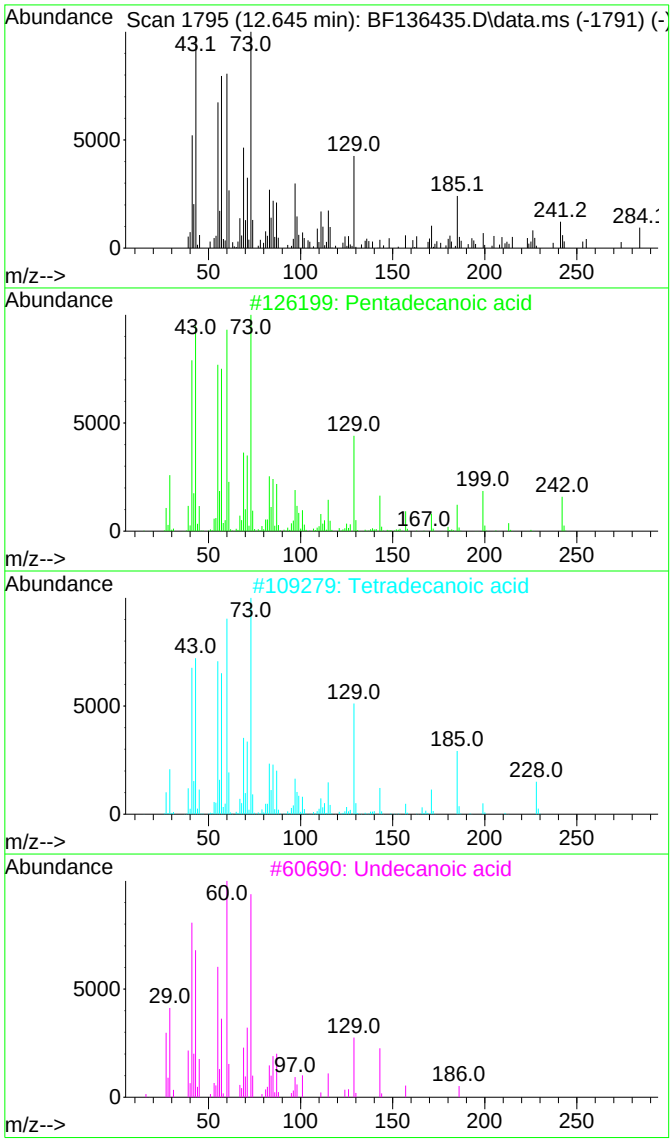
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

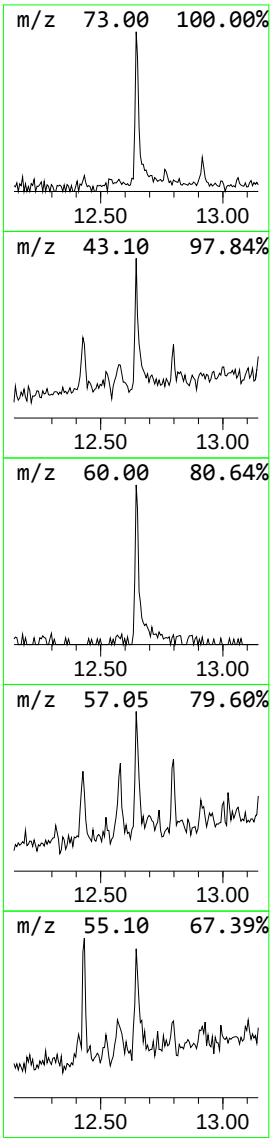
****

Peak Number 7 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	3.58 ng	95262	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Undecanoic acid	186	C11H22O2	000112-37-8	78
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5	Tridecanoic acid	214	C13H26O2	000638-53-9	59





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-11162023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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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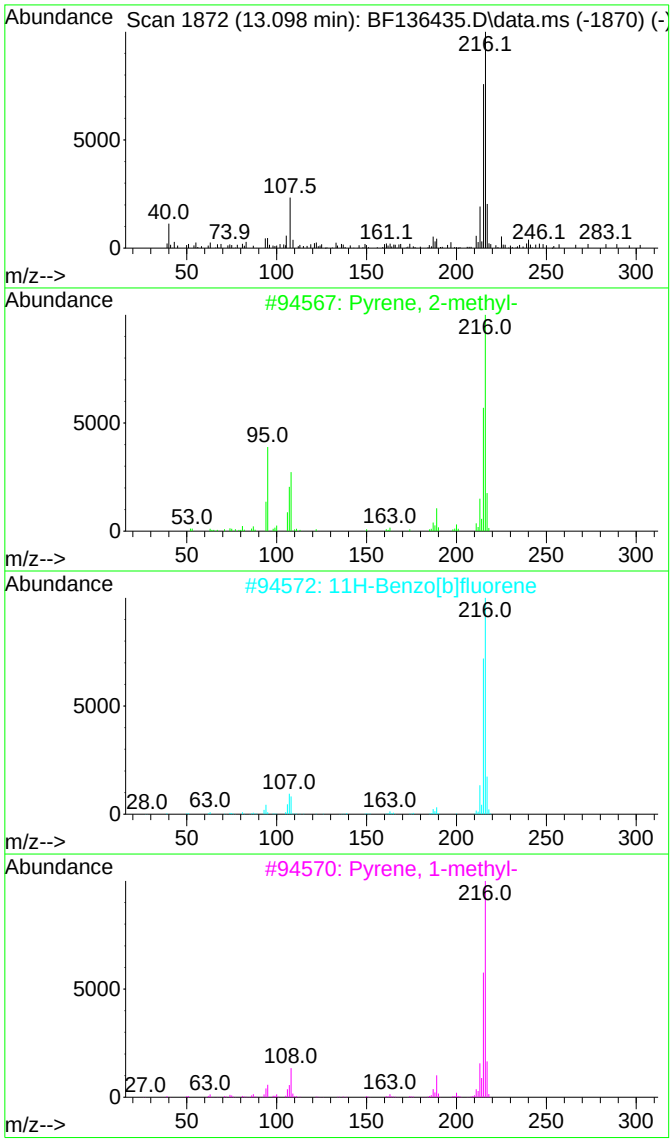
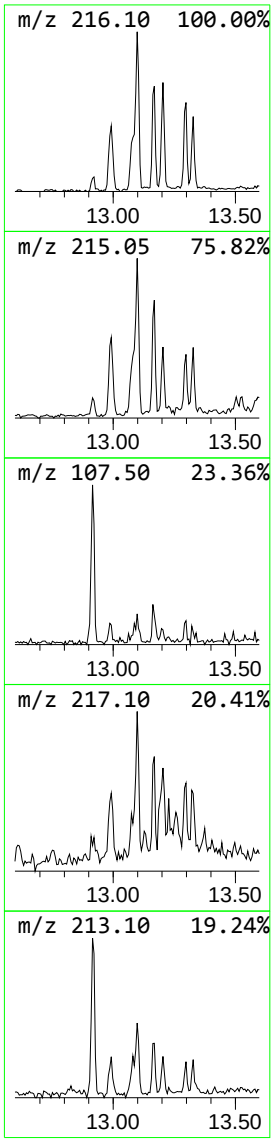
Peak Number 8 Pyrene, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.098	2.04 ng	62078	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 2-methyl-	216	C17H12	003442-78-2	90
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
4	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	80
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136435.D
Acq On : 06 Dec 2023 18:48
Operator : CG\JU
Sample : 05463-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-11162023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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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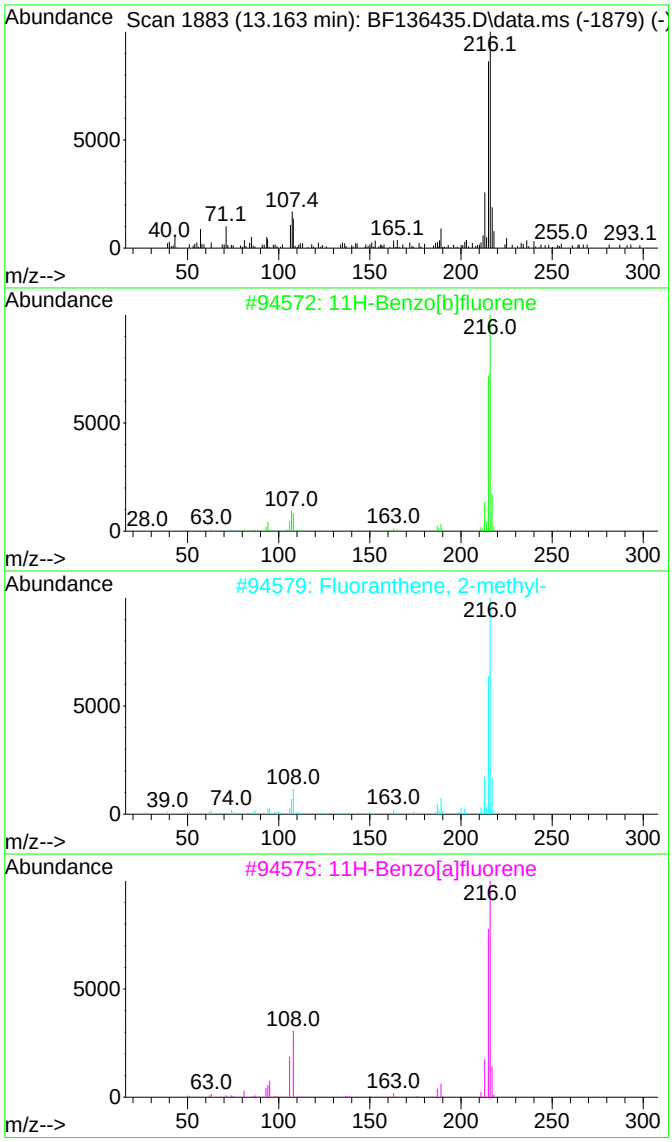
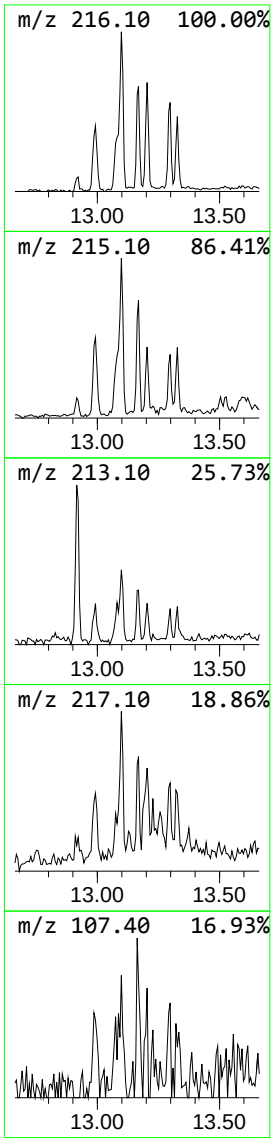
Peak Number 9 11H-Benzo[b]fluorene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.163	2.32 ng	70676	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
4	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136435.D
Acq On : 06 Dec 2023 18:48
Operator : CG\JU
Sample : 05463-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-11162023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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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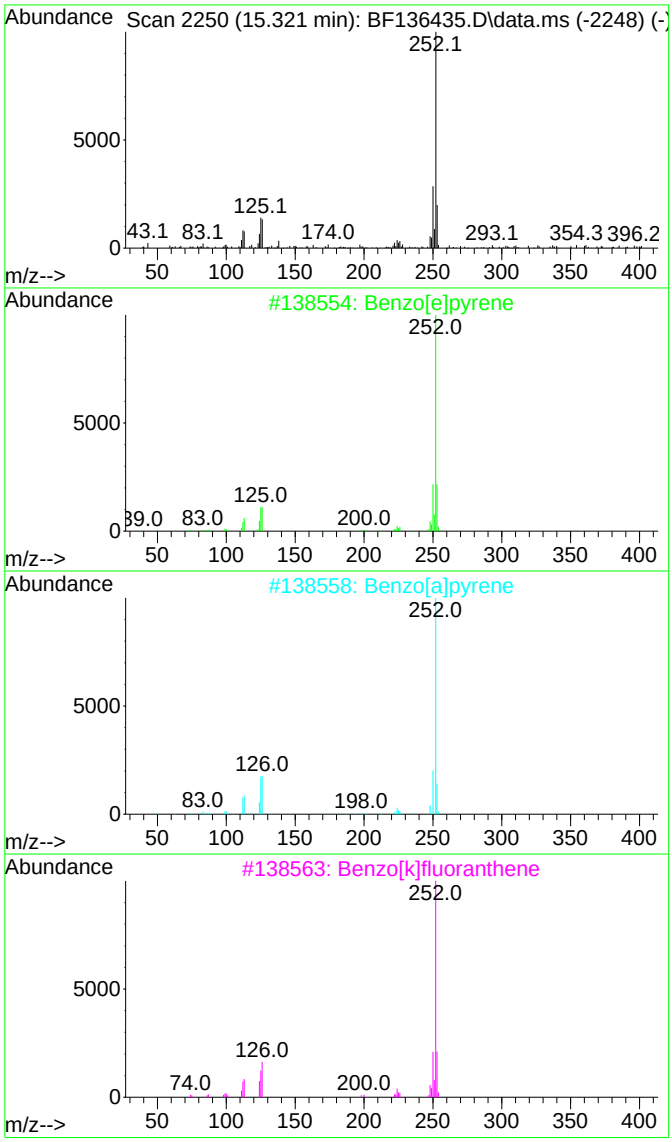
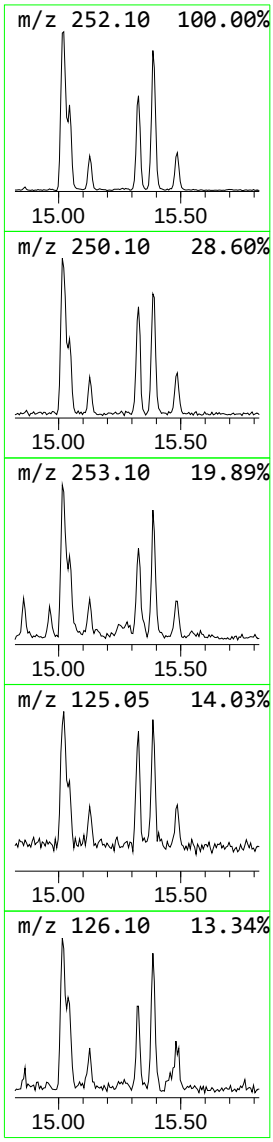
Peak Number 10 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.321	7.57 ng	118237	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	95
2	Benzo[a]pyrene	252	C20H12	000050-32-8	93
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136435.D
Acq On : 06 Dec 2023 18:48
Operator : CG\JU
Sample : 05463-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-11162023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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-...	5.034	6.5	ng	148242	1	6.798	452619	20.0
Dodecane, 2,6,1...	9.098	2.1	ng	51469	3	9.828	495646	20.0
2,4,7,9-Tetrame...	9.275	19.6	ng	484723	3	9.828	495646	20.0
n-Hexadecanoic ...	11.857	7.3	ng	195124	4	11.322	532881	20.0
4H-Cyclopenta[d...	11.933	3.1	ng	82002	4	11.322	532881	20.0
trans-13-Octade...	12.433	2.3	ng	60219	4	11.322	532881	20.0
Pentadecanoic acid	12.645	3.6	ng	95262	4	11.322	532881	20.0
Pyrene, 2-methyl-	13.098	2.0	ng	62078	5	13.974	608963	20.0
11H-Benzo[b]flu...	13.163	2.3	ng	70676	5	13.974	608963	20.0
Benzo[e]pyrene	15.321	7.6	ng	118237	6	15.457	312388	20.0