LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081623\
Data File : BF134799.D
Acq On : 16 Aug 2023 09:57
Operator : CG\JU
Sample : 04017-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : JC-03-081423-A

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-BF080123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134799.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.428	563	568	571	rBV	2401275	2274934	88.21%	9.742%
2	6.434	734	739	742	rBV	2200600	2227243	86.36%	9.538%
3	6.628	769	772	776	rBV	26258	29950	1.16%	0.128%
4	6.798	797	801	804	rBV	1252944	965938	37.45%	4.137%
5	7.357	892	896	899	rBV	1764563	1415332	54.88%	6.061%
6	8.075	1014	1018	1022	rBV	1486769	1219233	47.27%	5.221%
7	9.151	1197	1201	1211	rBV	2835366	2579067	100.00%	11.045%
8	9.233	1212	1215	1218	rVV3	33488	44721	1.73%	0.192%
9	9.269	1219	1221	1225	rVB	42148	42517	1.65%	0.182%
10	9.539	1264	1267	1268	rBV2	42046	30426	1.18%	0.130%
11	9.692	1291	1293	1297	rBV3	47192	53714	2.08%	0.230%
12	9.739	1299	1301	1304	rVB2	49458	41335	1.60%	0.177%
13	9.769	1304	1306	1310	rBV3	27085	31565	1.22%	0.135%
14	9.833	1310	1317	1320	rBV	1441306	1259951	48.85%	5.396%
15	9.863	1320	1322	1326	rVB	57489	56591	2.19%	0.242%
16	10.033	1348	1351	1354	rBV3	49896	52723	2.04%	0.226%
17	10.151	1368	1371	1372	rBV2	35911	30934	1.20%	0.132%
18	10.239	1383	1386	1388	rBV2	41154	37999	1.47%	0.163%
19	10.269	1388	1391	1393	rVB2	37604	32383	1.26%	0.139%
20	10.375	1407	1409	1412	rBV2	61514	68555	2.66%	0.294%
21	10.492	1426	1429	1433	rVB2	74503	67423	2.61%	0.289%
22	10.539	1435	1437	1441	rVB3	47800	54995	2.13%	0.236%
23	10.580	1441	1444	1446	rBV4	35878	39278	1.52%	0.168%
24	10.622	1447	1451	1455	rBV	1449512	1264644	49.03%	5.416%
25	10.757	1469	1474	1479	rBV2	119354	183988	7.13%	0.788%
26	11.192	1546	1548	1550	rBV	42189	36770	1.43%	0.157%
27	11.222	1550	1553	1559	rVB2	154536	170828	6.62%	0.732%
28	11.322	1566	1570	1572	rBV	1205653	992243	38.47%	4.249%
29	11.345	1572	1574	1577	rVV	610455	474822	18.41%	2.033%
30	11.392	1580	1582	1586	rVB	111747	108354	4.20%	0.464%
31	11.622	1619	1621	1624	rVB	57964	40084	1.55%	0.172%
32	11.827	1653	1656	1657	rBV	80494	74963	2.91%	0.321%
33	11.857	1658	1661	1665	rVB	459858	401414	15.56%	1.719%
34	11.933	1672	1674	1677	rBV	123702	116827	4.53%	0.500%
35	12.122	1704	1706	1708	rBV	64231	55828	2.16%	0.239%
36	12.374	1747	1749	1752	rBV	118729	120459	4.67%	0.516%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081623\
Data File : BF134799.D
Acq On : 16 Aug 2023 09:57
Operator : CG\JU
Sample : 04017-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-03-081423-A

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-BF080123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.410	1753	1755	1758	rBV4	136497	151687	5.88%	0.650%
38	12.539	1773	1777	1780	rBV	814608	701531	27.20%	3.004%
39	12.645	1792	1795	1798	rBV5	107174	110112	4.27%	0.472%
40	12.769	1811	1816	1819	rBV	842537	808637	31.35%	3.463%
41	12.916	1837	1841	1848	rVB	2300101	2061420	79.93%	8.828%
42	13.098	1870	1872	1875	rVB	183134	159964	6.20%	0.685%
43	13.204	1887	1890	1897	rBV	139854	190120	7.37%	0.814%
44	13.968	2016	2020	2023	rBV2	963550	1208905	46.87%	5.177%
45	13.998	2023	2025	2027	rVB	312356	230689	8.94%	0.988%
46	15.015	2195	2198	2201	rBV	199032	283982	11.01%	1.216%
47	15.380	2257	2260	2266	rBV	152532	206825	8.02%	0.886%
48	15.445	2267	2271	2275	rBV	442245	539029	20.90%	2.308%

Sum of corrected areas: 23350932

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Instrument :
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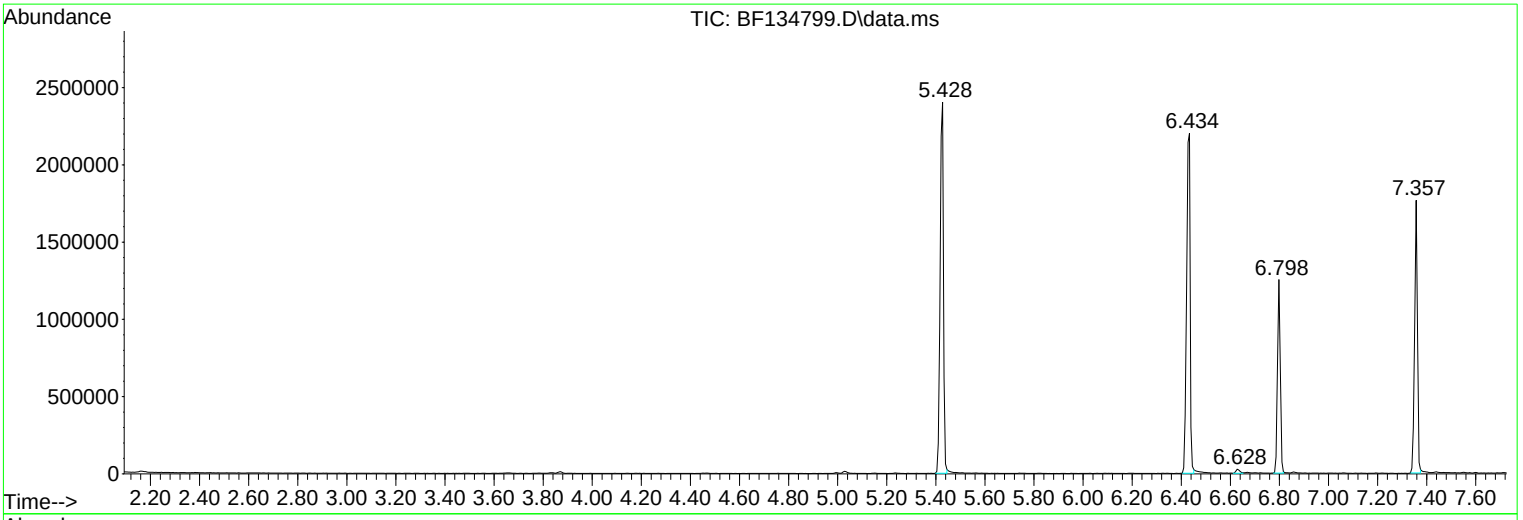
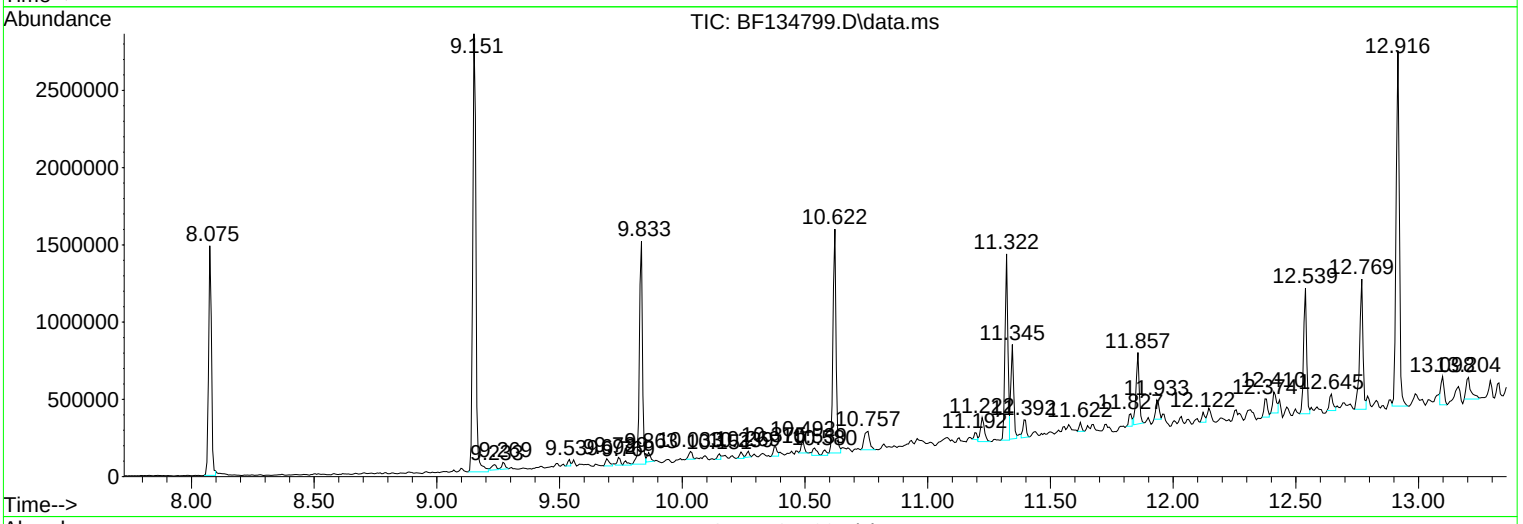
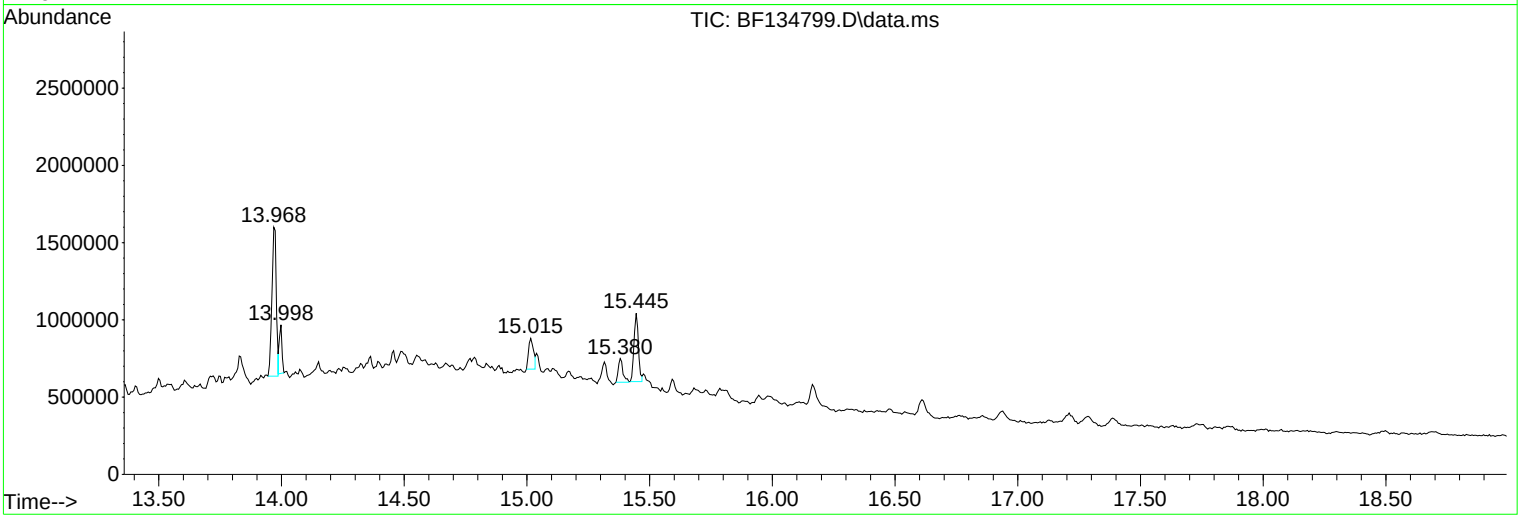
ClientSampleId :
JC-03-081423-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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\BF081623\
Data File : BF134799.D
Acq On : 16 Aug 2023 09:57
Operator : CG\JU
Sample : 04017-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-03-081423-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

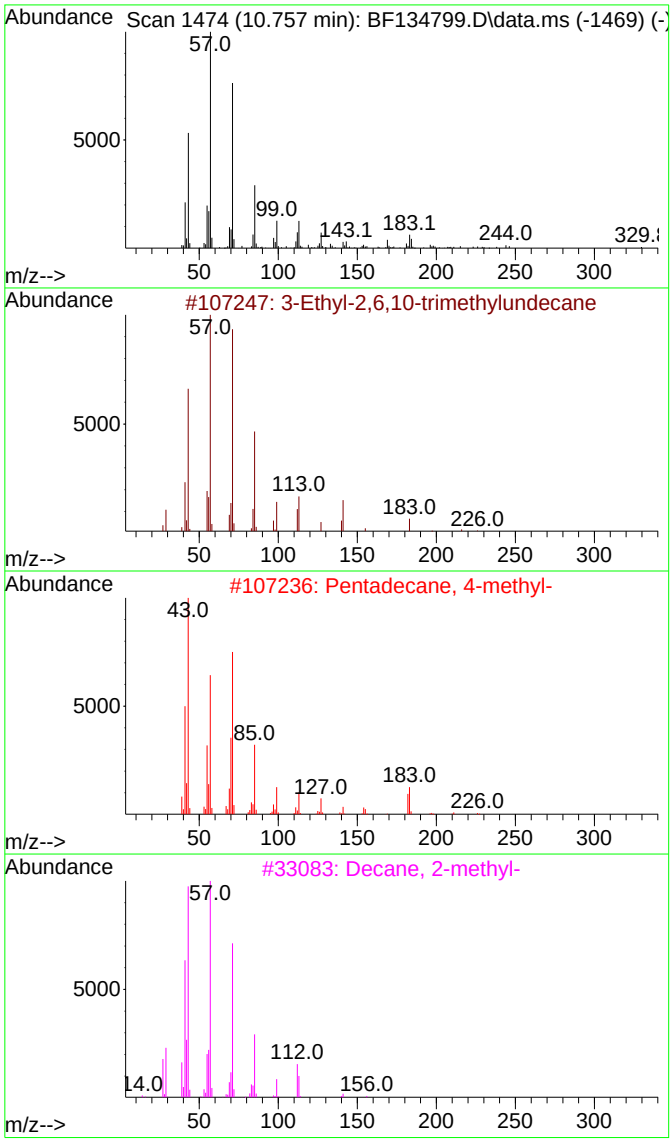
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

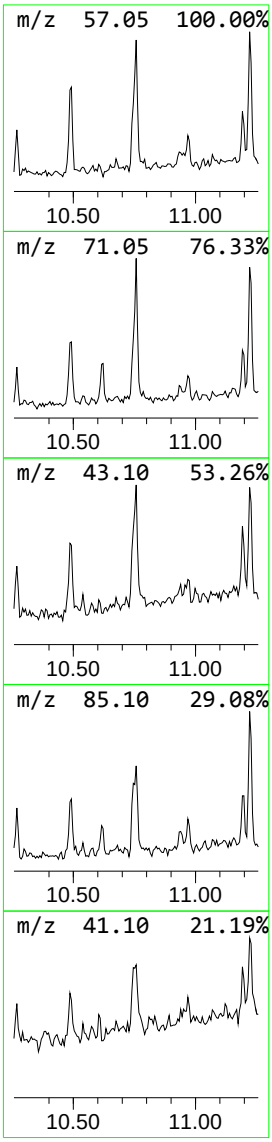
****

Peak Number 1 3-Ethyl-2,6,10-trimethylund... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.757	3.71 ng	183988	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Ethyl-2,6,10-trimethylundecane	226	C16H34	1000432-25-9	93
2	Pentadecane, 4-methyl-	226	C16H34	002801-87-8	91
3	Decane, 2-methyl-	156	C11H24	006975-98-0	87
4	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	83
5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081623\
Data File : BF134799.D
Acq On : 16 Aug 2023 09:57
Operator : CG\JU
Sample : 04017-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-03-081423-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

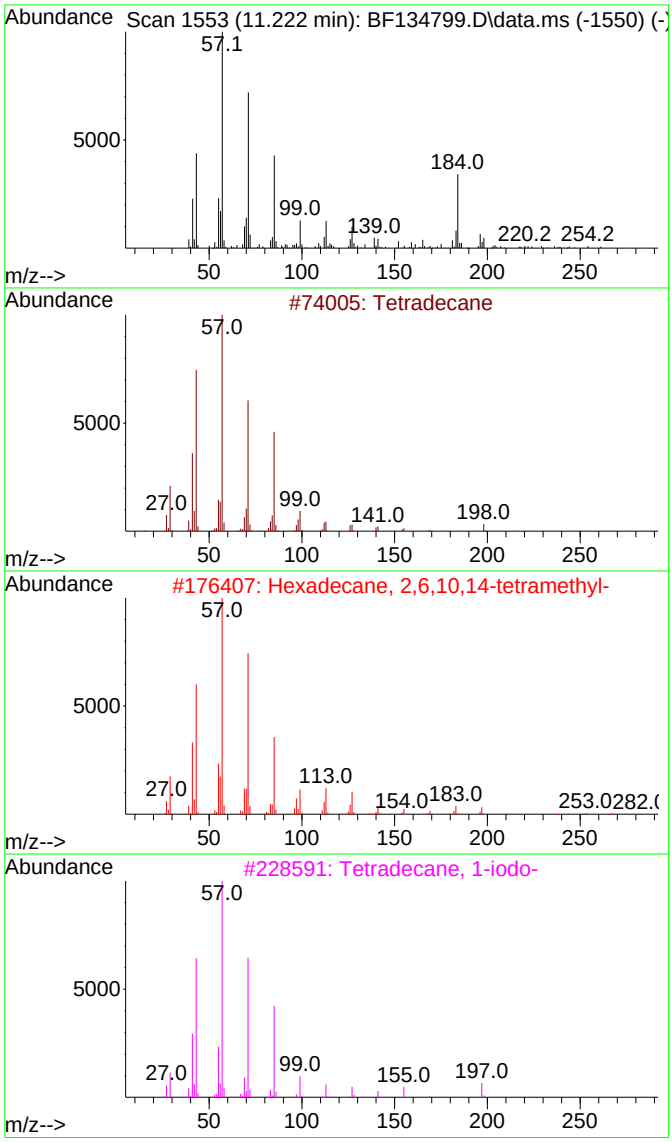
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

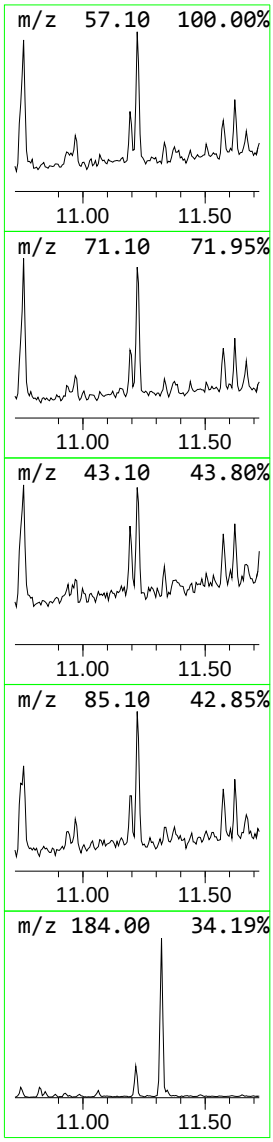
****

Peak Number 2 Tetradecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.222	3.44 ng	170828	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	76
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	74
3	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72
4	Octadecane	254	C18H38	000593-45-3	72
5	Dodecane, 5,8-diethyl-	226	C16H34	024251-86-3	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081623\
Data File : BF134799.D
Acq On : 16 Aug 2023 09:57
Operator : CG\JU
Sample : 04017-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-03-081423-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

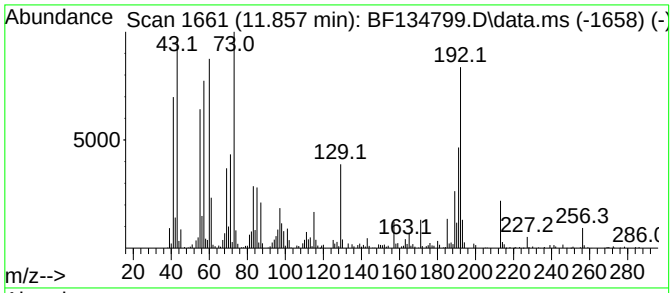
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

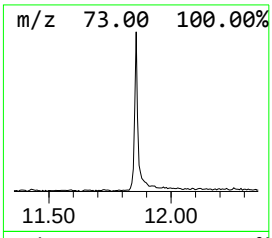
****

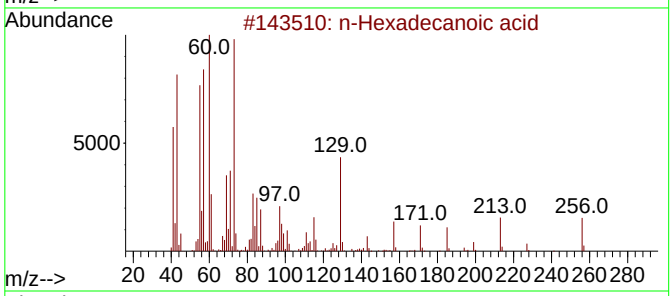
Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

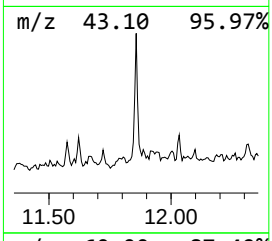
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	8.09 ng	401414	Phenanthrene-d10	11.322

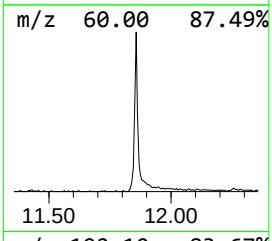
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	81
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	66
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	56

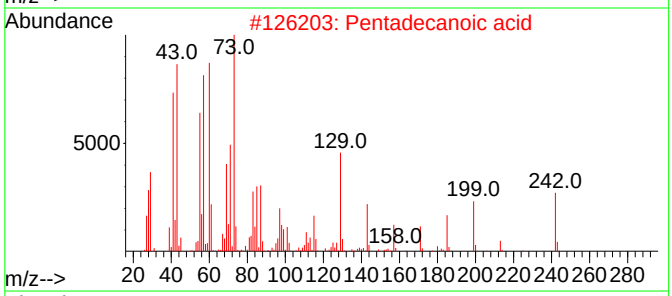


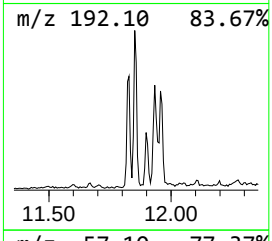


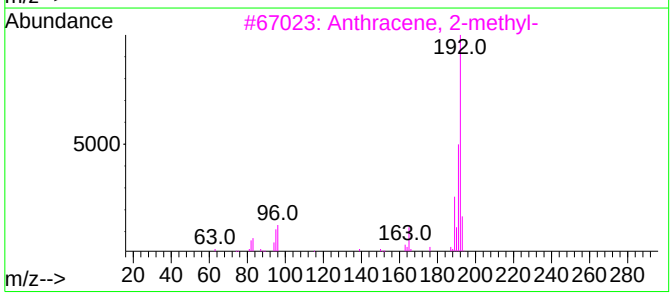


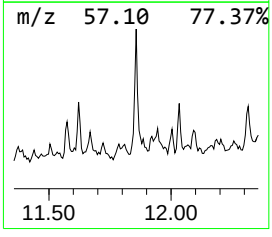












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Data File : BF134799.D
Acq On : 16 Aug 2023 09:57
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Misc :
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Instrument :
BNA_F
ClientSampleId :
JC-03-081423-A

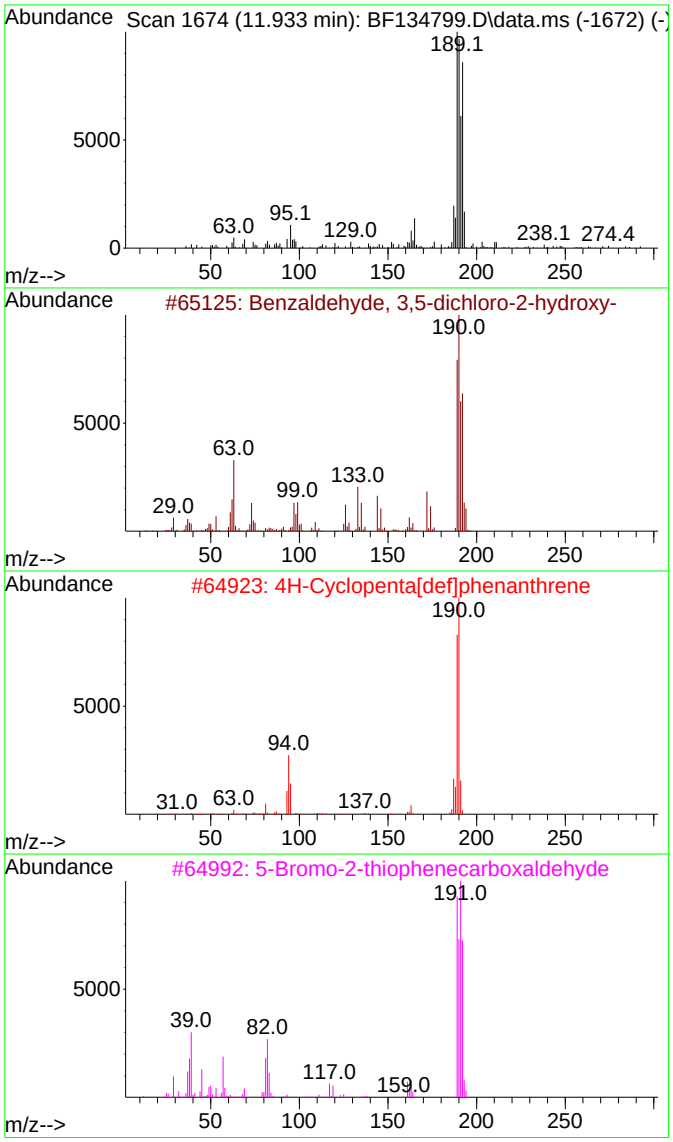
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

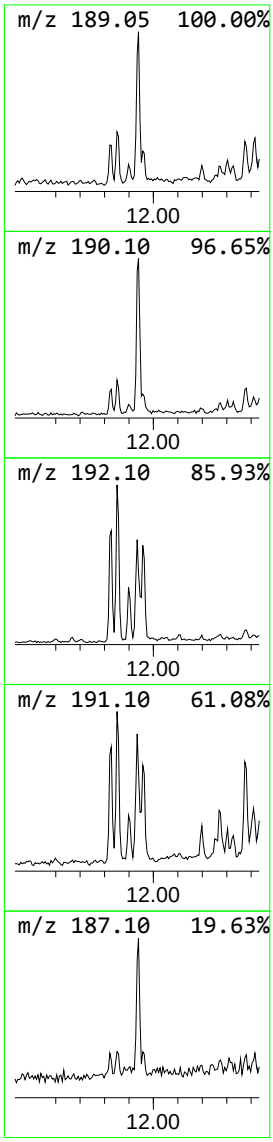
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzaldehyde, 3,5-dichloro-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	2.35 ng	116827	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	80
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	53
3	5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	53
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	46
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	41





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Data File : BF134799.D
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Sample : 04017-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-03-081423-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

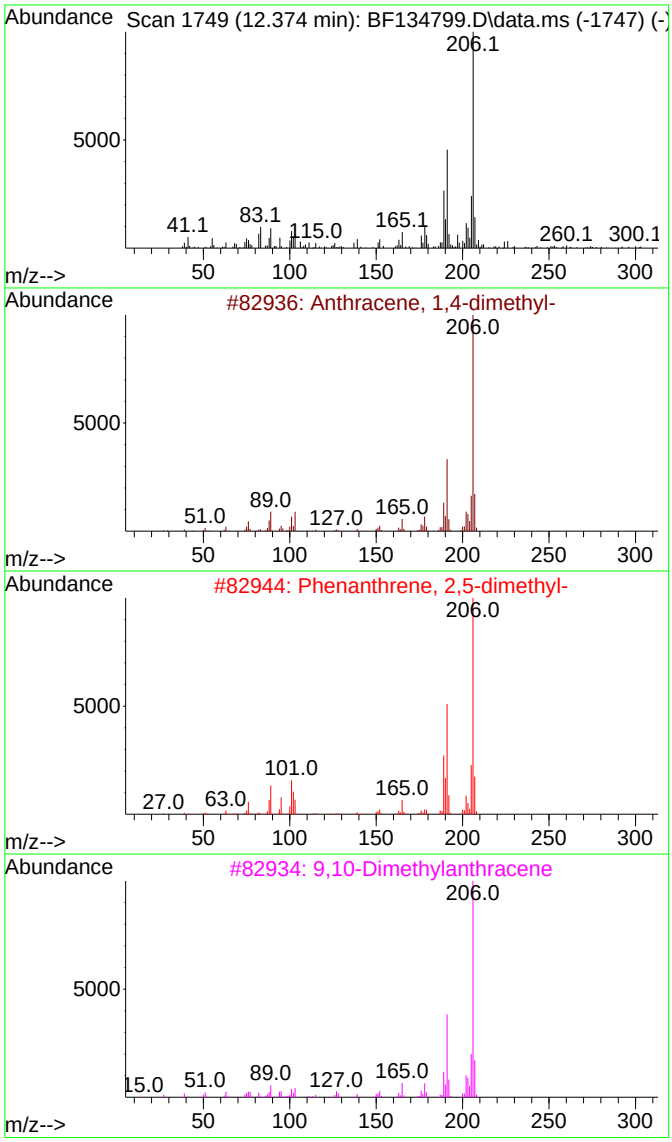
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

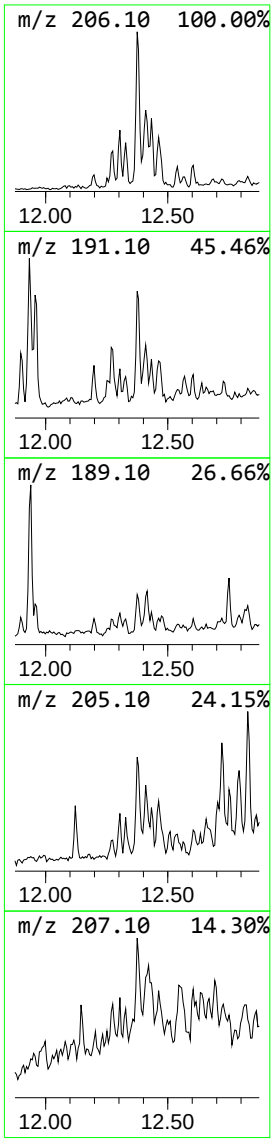
****

Peak Number 5 Anthracene, 1,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.374	2.43 ng	120459	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	93
2	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
3	9,10-Dimethylanthracene	206	C16H14	000781-43-1	93
4	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	93
5	di-p-Tolylacetylene	206	C16H14	002789-88-0	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081623\
Data File : BF134799.D
Acq On : 16 Aug 2023 09:57
Operator : CG\JU
Sample : 04017-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-03-081423-A

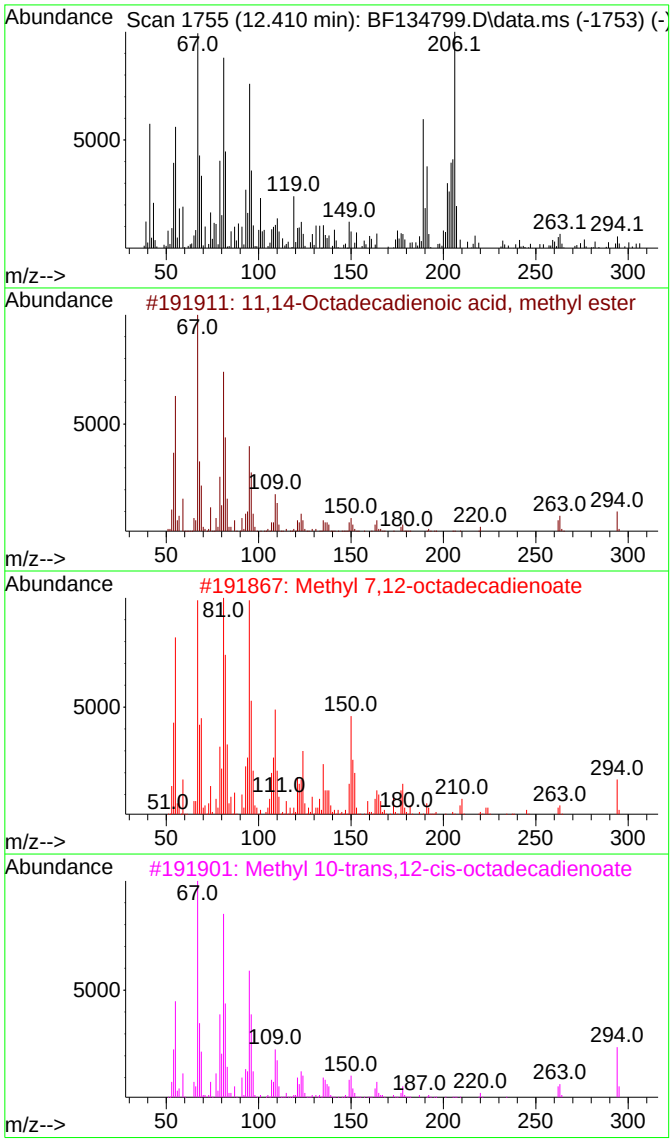
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

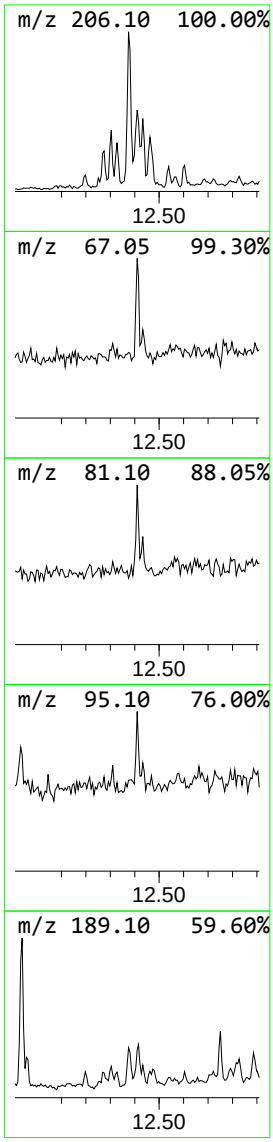
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 11,14-Octadecadienoic acid,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	3.06 ng	151687	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	80
2	Methyl 7,12-octadecadienoate	294	C19H34O2	1000336-43-8	55
3	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	52
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	45
5	12,15-Octadecadienoic acid, meth...	294	C19H34O2	057156-97-5	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081623\
Data File : BF134799.D
Acq On : 16 Aug 2023 09:57
Operator : CG\JU
Sample : 04017-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-03-081423-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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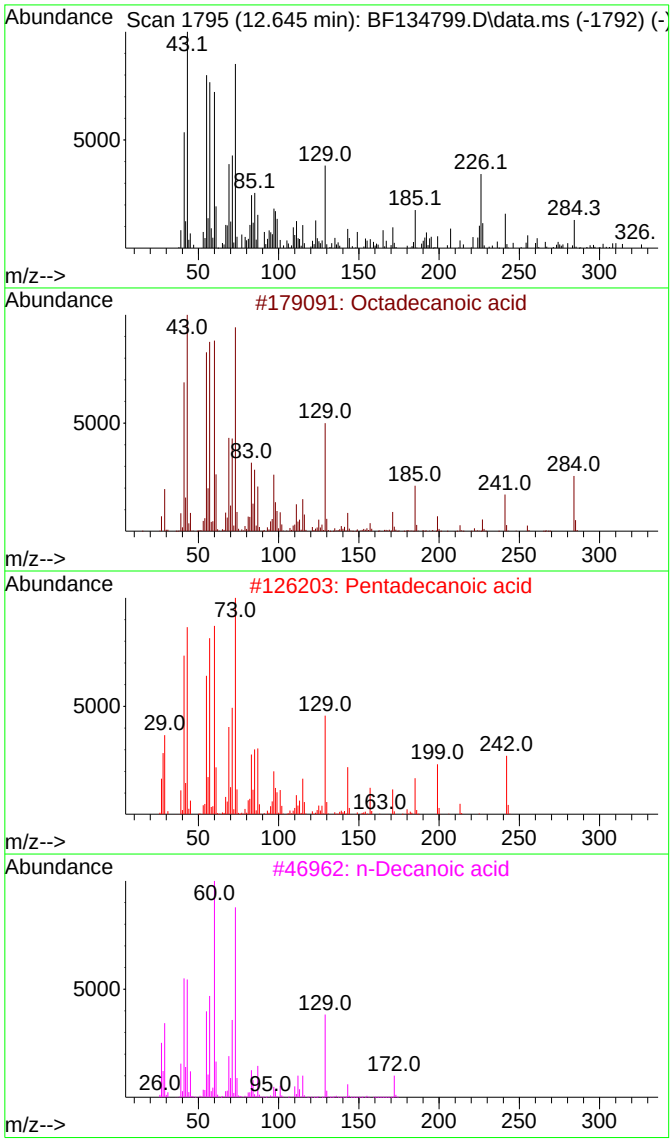
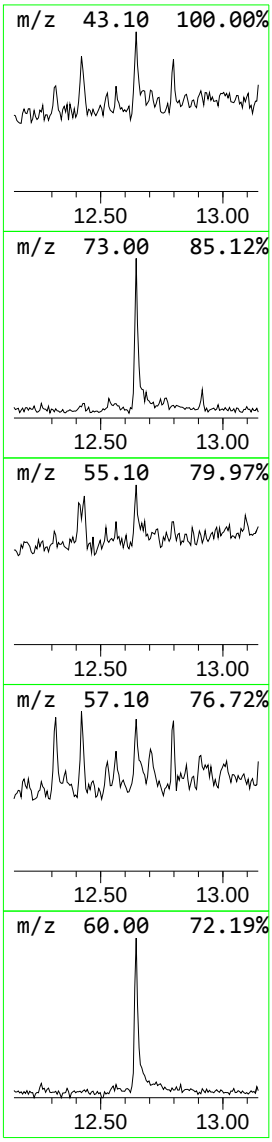
Peak Number 7 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	2.22 ng	110112	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081623\
Data File : BF134799.D
Acq On : 16 Aug 2023 09:57
Operator : CG\JU
Sample : 04017-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-03-081423-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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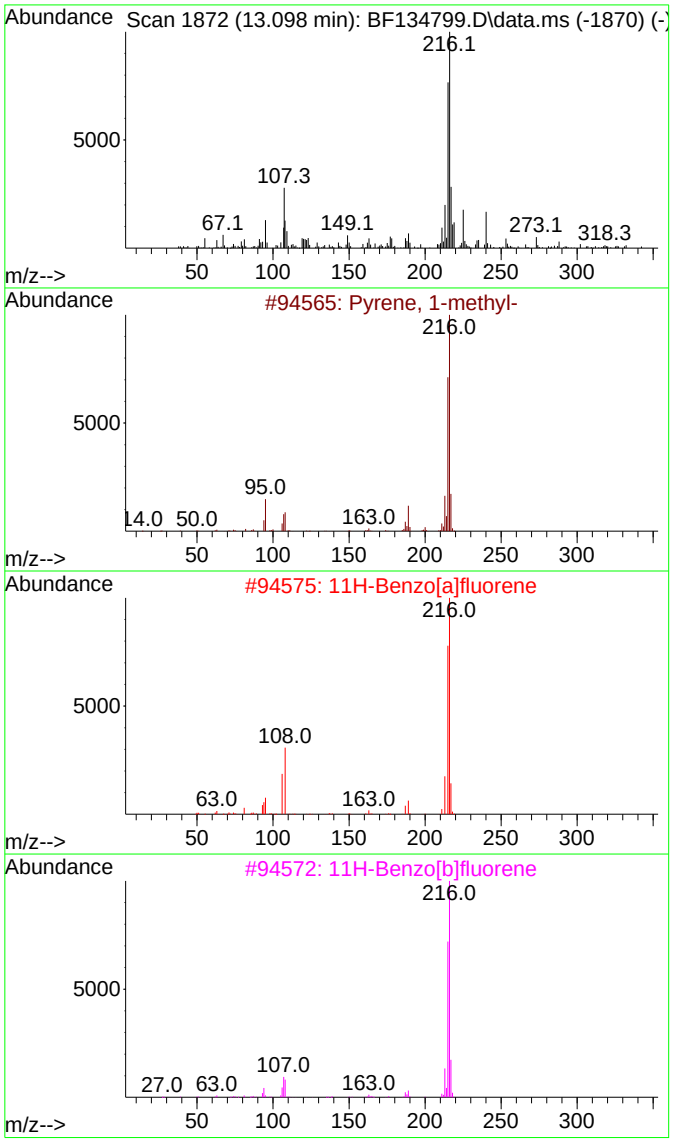
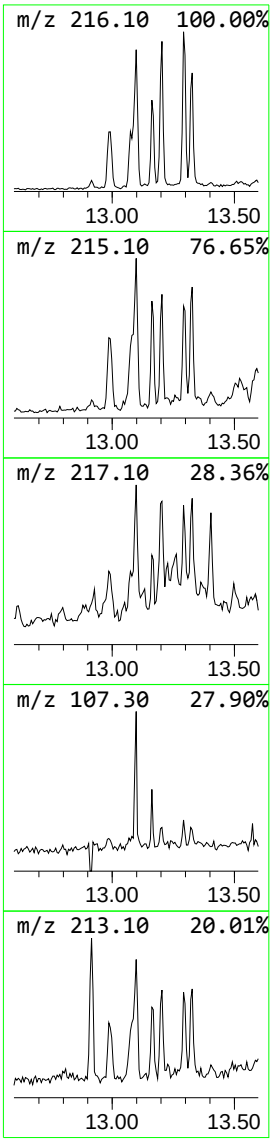
Peak Number 8 Pyrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.098	2.65 ng	159964	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	68
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	64
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	64
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	52
5	2,4-Dichloro-6,7,8,9-tetrahydro-...	216	C9H10Cl2N2	076780-96-6	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081623\
Data File : BF134799.D
Acq On : 16 Aug 2023 09:57
Operator : CG\JU
Sample : 04017-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-03-081423-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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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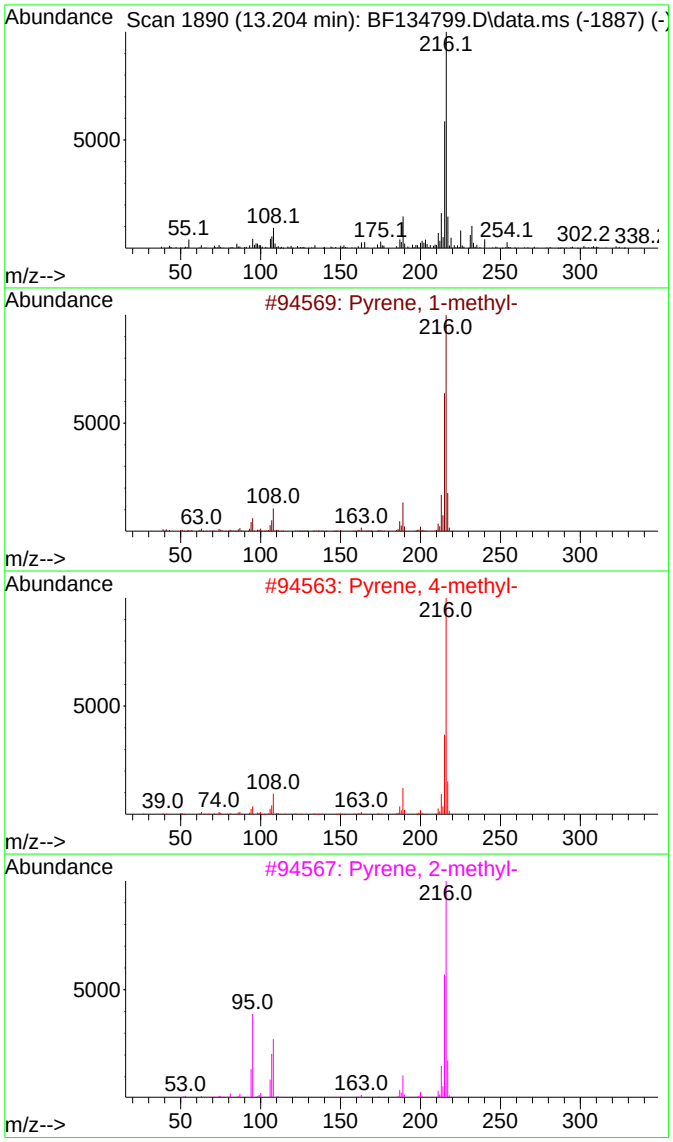
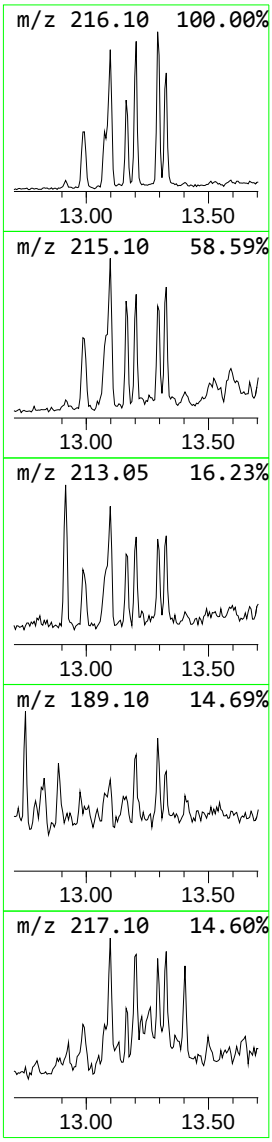
Peak Number 9 Pyrene, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.204	3.15 ng	190120	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	95
2	Pyrene, 4-methyl-	216	C17H12	003353-12-6	94
3	Pyrene, 2-methyl-	216	C17H12	003442-78-2	93
4	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	83
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081623\
Data File : BF134799.D
Acq On : 16 Aug 2023 09:57
Operator : CG\JU
Sample : 04017-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-03-081423-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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
3-Ethyl-2,6,10-...	10.757	3.7	ng	183988	4	11.322	992243	20.0
Tetradecane	11.222	3.4	ng	170828	4	11.322	992243	20.0
n-Hexadecanoic ...	11.857	8.1	ng	401414	4	11.322	992243	20.0
Benzaldehyde, 3...	11.933	2.4	ng	116827	4	11.322	992243	20.0
Anthracene, 1,4...	12.374	2.4	ng	120459	4	11.322	992243	20.0
11,14-Octadecad...	12.410	3.1	ng	151687	4	11.322	992243	20.0
Octadecanoic acid	12.645	2.2	ng	110112	4	11.322	992243	20.0
Pyrene, 1-methyl-	13.098	2.6	ng	159964	5	13.974	1208910	20.0
Pyrene, 4-methyl-	13.204	3.1	ng	190120	5	13.974	1208910	20.0