LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
Data File : BF133251.D
Acq On : 05 May 2023 01:44
Operator : CG\JU
Sample : 02588-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ZONE-B-0-3-05012023

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133251.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.716	271	277	282	rVB	84560	121316	2.98%	0.347%
2	4.922	474	482	490	rBV	78924	110732	2.72%	0.316%
3	5.340	548	553	556	rBV	3969734	3841066	94.30%	10.973%
4	6.363	722	727	730	rBV	3621124	3845069	94.40%	10.985%
5	6.722	785	788	792	rBV	1301022	1115572	27.39%	3.187%
6	7.140	852	859	867	rBV	49346	62680	1.54%	0.179%
7	7.292	880	885	887	rBV	2763705	2550581	62.62%	7.286%
8	8.010	1003	1007	1010	rBV	1991703	1501839	36.87%	4.290%
9	9.087	1186	1190	1193	rBV	5049949	4073108	100.00%	11.636%
10	9.757	1301	1304	1307	rBV	1907351	1563067	38.38%	4.465%
11	9.792	1307	1310	1314	rVB	131004	114607	2.81%	0.327%
12	9.963	1335	1339	1344	rBV	70892	66980	1.64%	0.191%
13	10.304	1394	1397	1400	rBV	142833	113580	2.79%	0.324%
14	10.469	1421	1425	1429	rVB	299890	269638	6.62%	0.770%
15	10.545	1434	1438	1442	rBV	2442741	2233077	54.82%	6.379%
16	11.133	1536	1538	1543	rVB	54278	61497	1.51%	0.176%
17	11.239	1552	1556	1558	rBV	1675893	1362946	33.46%	3.894%
18	11.263	1558	1560	1563	rVV	1017766	763373	18.74%	2.181%
19	11.316	1565	1569	1572	rVB	258136	233000	5.72%	0.666%
20	11.739	1638	1641	1644	rBV	88504	82679	2.03%	0.236%
21	11.775	1644	1647	1651	rVV2	265195	296580	7.28%	0.847%
22	11.816	1651	1654	1657	rVB2	53841	53253	1.31%	0.152%
23	11.851	1657	1660	1663	rBV	188640	185785	4.56%	0.531%
24	12.039	1689	1692	1693	rBV	62692	50646	1.24%	0.145%
25	12.292	1732	1735	1737	rBV	64485	60709	1.49%	0.173%
26	12.375	1746	1749	1754	rBV3	31137	50523	1.24%	0.144%
27	12.451	1758	1762	1765	rVV	1289106	1065911	26.17%	3.045%
28	12.498	1767	1770	1776	rVB5	49906	73553	1.81%	0.210%
29	12.675	1795	1800	1803	rBV	957337	1010236	24.80%	2.886%
30	12.798	1818	1821	1822	rBV	65805	53036	1.30%	0.152%
31	12.827	1822	1826	1829	rVV	3274267	2840632	69.74%	8.115%
32	13.004	1854	1856	1860	rVB	166124	158954	3.90%	0.454%
33	13.074	1864	1868	1870	rBV2	180684	178463	4.38%	0.510%
34	13.110	1871	1874	1876	rBV	97441	89314	2.19%	0.255%
35	13.233	1892	1895	1899	rBV	50404	62574	1.54%	0.179%
36	13.410	1923	1925	1927	rBV	64725	48709	1.20%	0.139%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
Data File : BF133251.D
Acq On : 05 May 2023 01:44
Operator : CG\JU
Sample : 02588-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ZONE-B-0-3-05012023

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.739	1978	1981	1987	rBV3	178320	226245	5.55%	0.646%
38	13.874	1999	2004	2006	rBV2	1269565	1504685	36.94%	4.299%
39	13.898	2006	2008	2011	rVB	471707	358102	8.79%	1.023%
40	13.980	2020	2022	2024	rVB	89664	65268	1.60%	0.186%
41	14.057	2032	2035	2038	rVB3	86856	96416	2.37%	0.275%
42	14.357	2083	2086	2088	rBV3	148124	136650	3.35%	0.390%
43	14.886	2173	2176	2179	rBV	325832	458502	11.26%	1.310%
44	15.174	2222	2225	2231	rVB	220955	261068	6.41%	0.746%
45	15.227	2231	2234	2241	rBV	265574	333698	8.19%	0.953%
46	15.292	2241	2245	2248	rBV	689413	805209	19.77%	2.300%
47	15.745	2319	2322	2327	rBV3	77617	119565	2.94%	0.342%
48	15.957	2355	2358	2371	rVB4	124853	273765	6.72%	0.782%

Sum of corrected areas: 35004458

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
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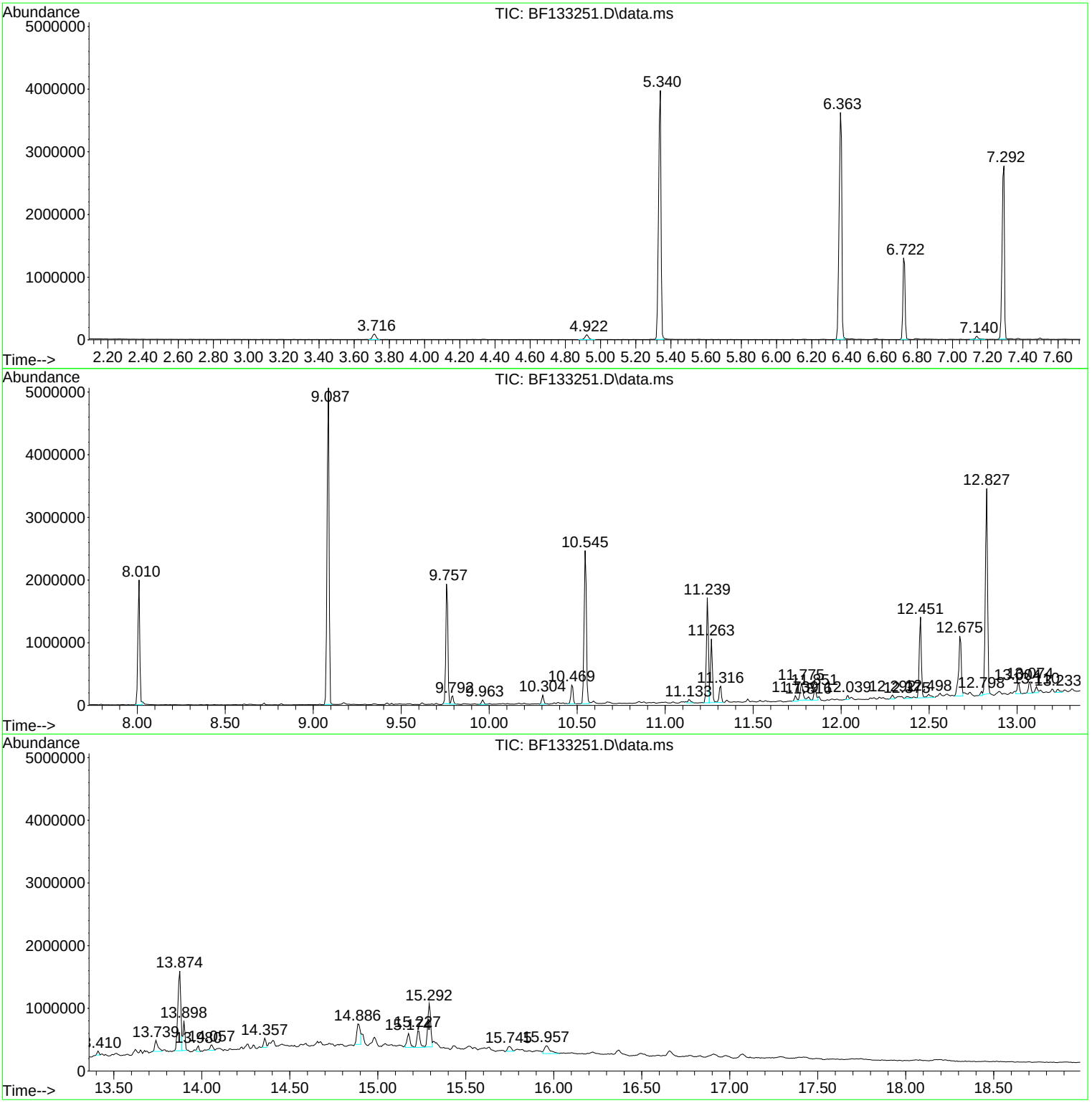
Instrument :
BNA_F
ClientSampleId :
ZONE-B-0-3-05012023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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\BF050423\
Data File : BF133251.D
Acq On : 05 May 2023 01:44
Operator : CG\JU
Sample : 02588-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ZONE-B-0-3-05012023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

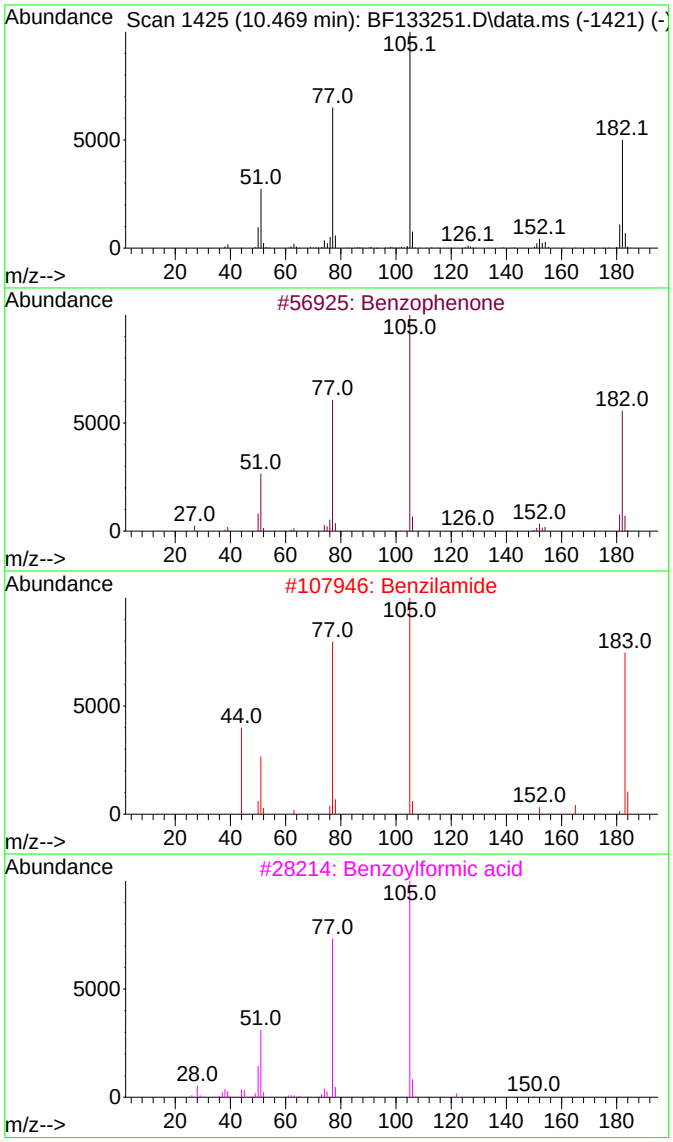
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

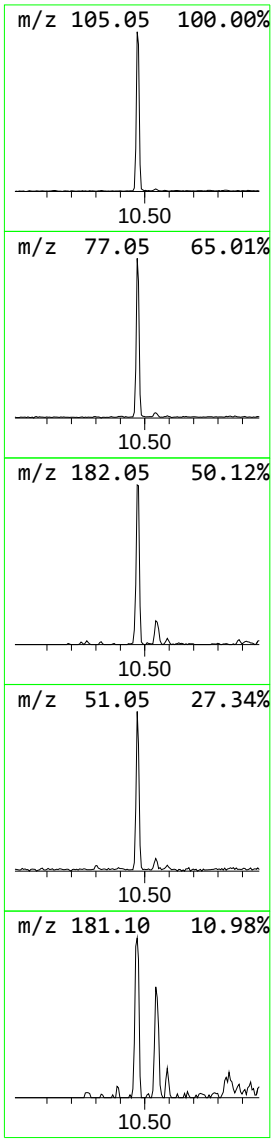
****

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.469	3.45 ng	269638	Acenaphthene-d10	9.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzilamide	227	C14H13NO2	004746-87-6	50
3	Benzoylformic acid	150	C8H6O3	000611-73-4	49
4	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	49
5	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
Data File : BF133251.D
Acq On : 05 May 2023 01:44
Operator : CG\JU
Sample : 02588-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ZONE-B-0-3-05012023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

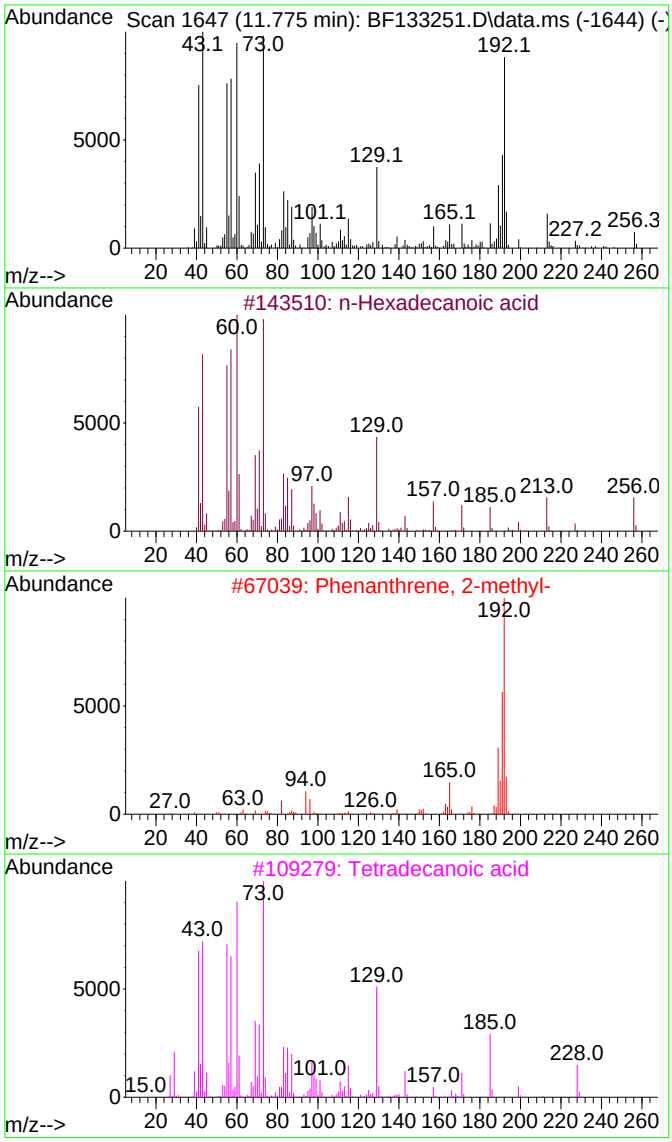
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

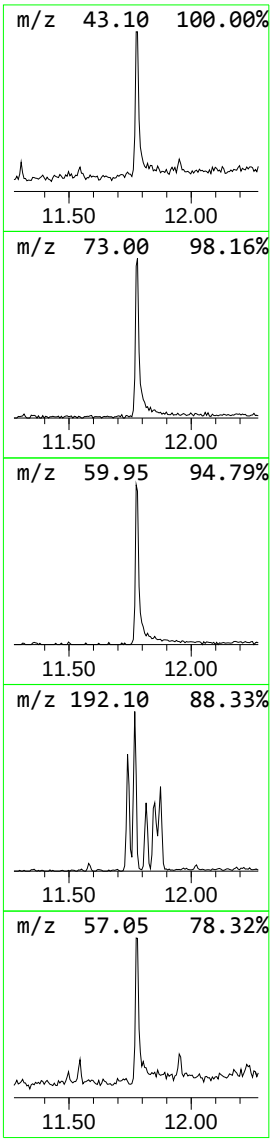
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.775	4.35 ng	296580	Phenanthrene-d10	11.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	78
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
Data File : BF133251.D
Acq On : 05 May 2023 01:44
Operator : CG\JU
Sample : 02588-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ZONE-B-0-3-05012023

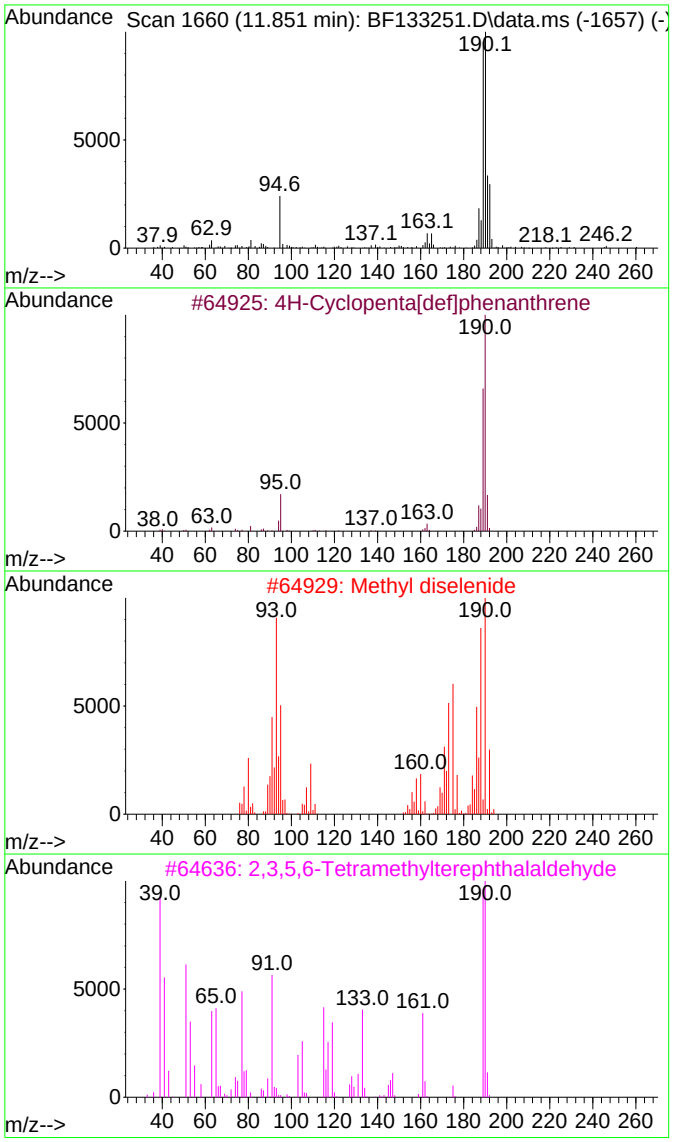
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

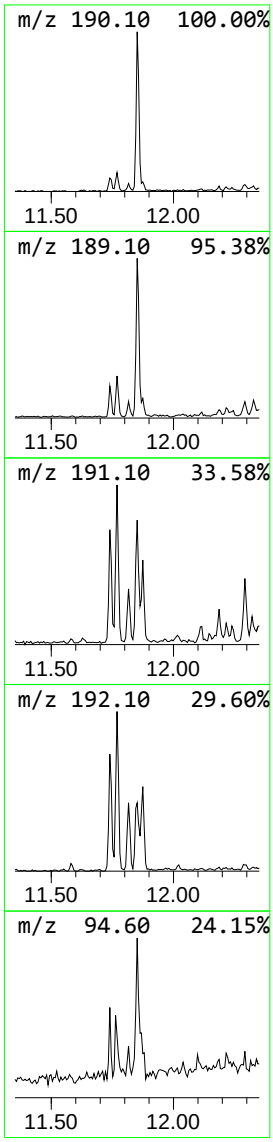
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	2.73 ng	185785	Phenanthrene-d10	11.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	Methyl diselenide	190	C2H6Se2	007101-31-7	55
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
5	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
Data File : BF133251.D
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Operator : CG\JU
Sample : 02588-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ZONE-B-0-3-05012023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

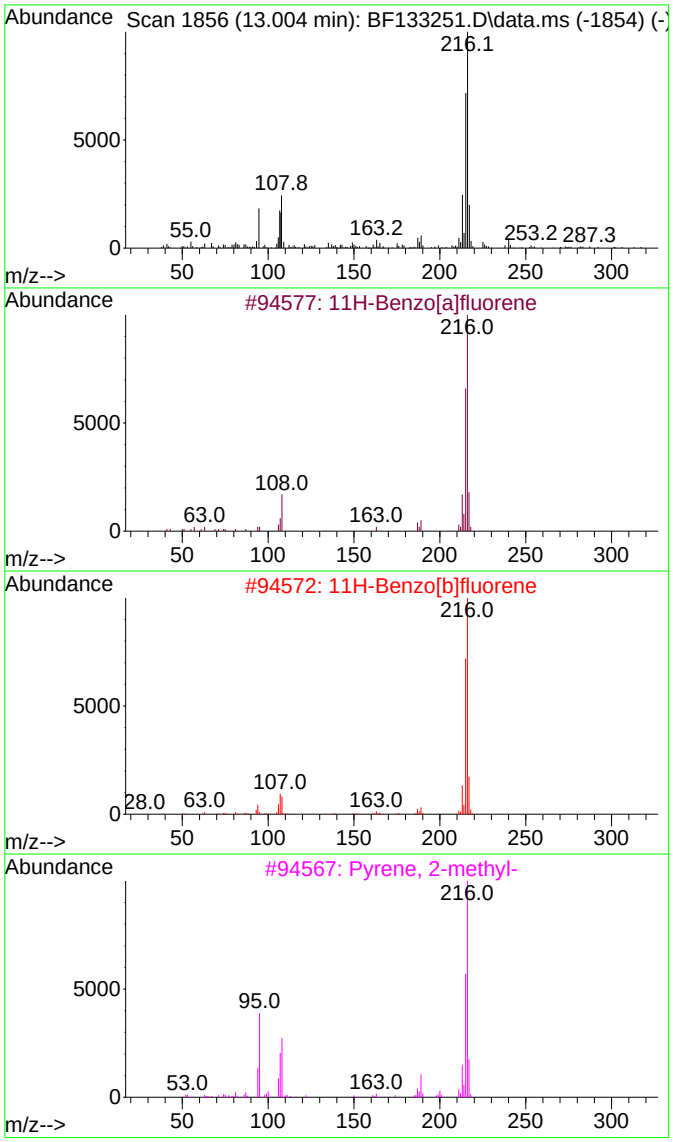
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

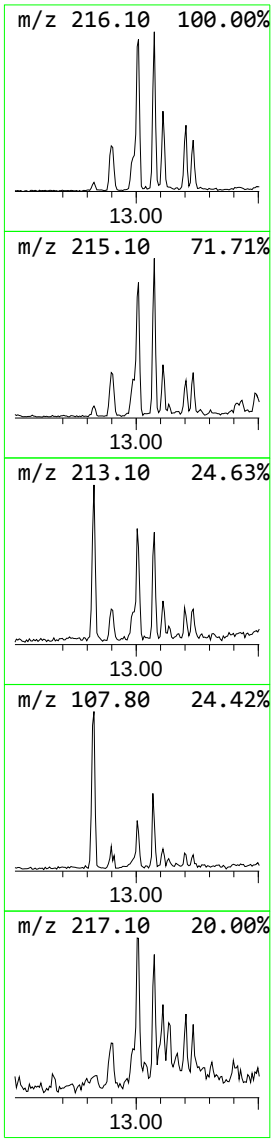
****

Peak Number 5 11H-Benzo[a]fluorene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.004	2.11 ng	158954	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
3	Pyrene, 2-methyl-	216	C17H12	003442-78-2	83
4	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	81
5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
Data File : BF133251.D
Acq On : 05 May 2023 01:44
Operator : CG\JU
Sample : 02588-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ZONE-B-0-3-05012023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

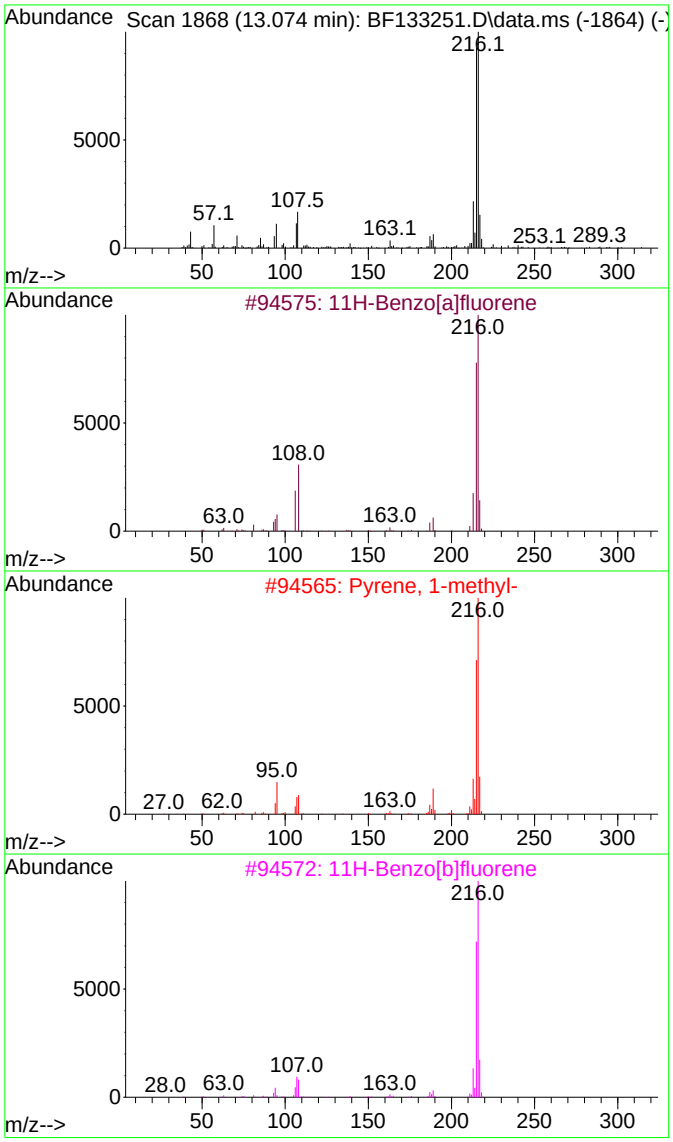
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

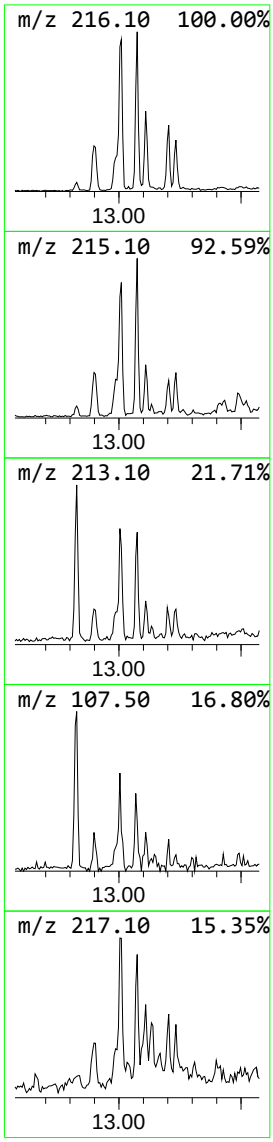
****

Peak Number 6 Pyrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.075	2.37 ng	178463	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	86
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	72
4	trans-p-(Trifluoromethyl)cinnami...	216	C10H7F3O2	016642-92-5	59
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	59





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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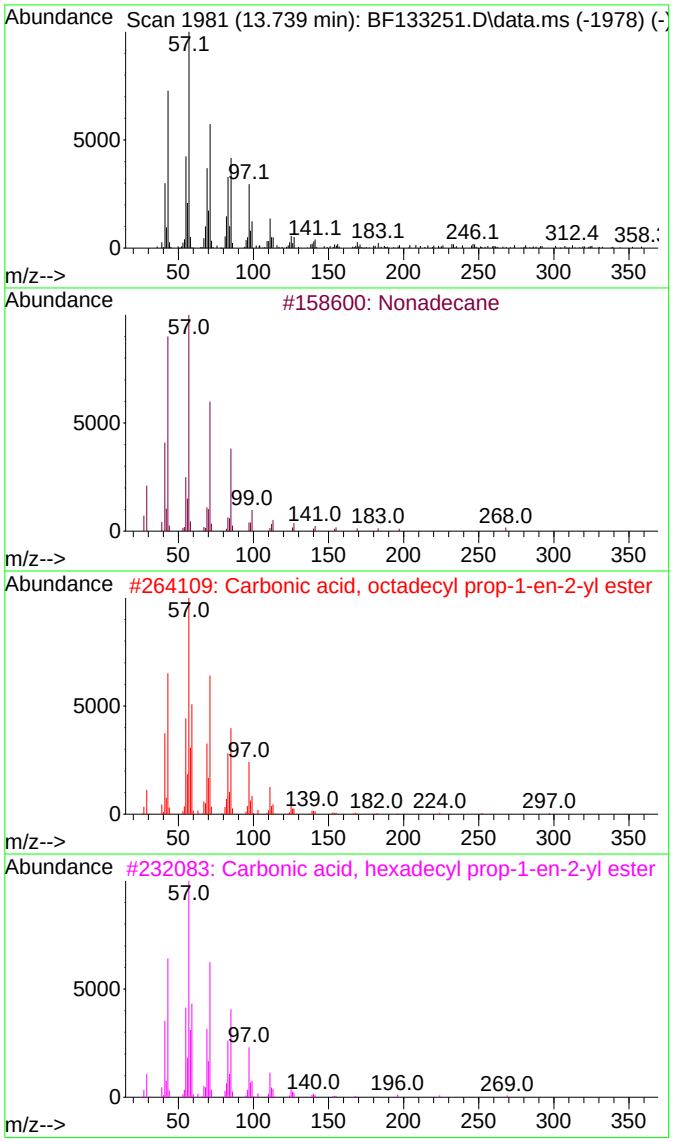
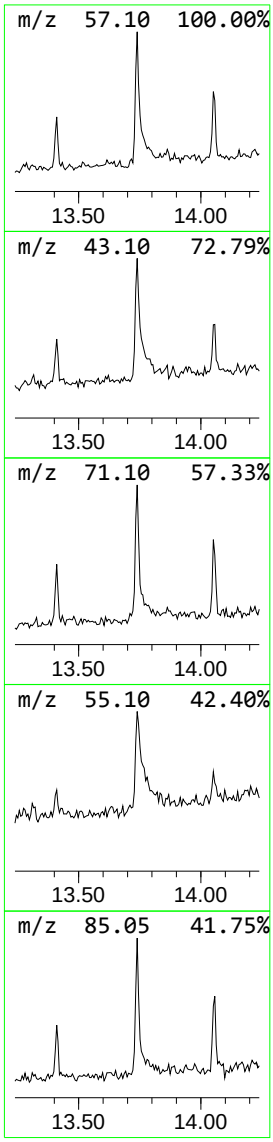
Peak Number 7 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	3.01 ng	226245	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
3	Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	91
4	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	91
5	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	90





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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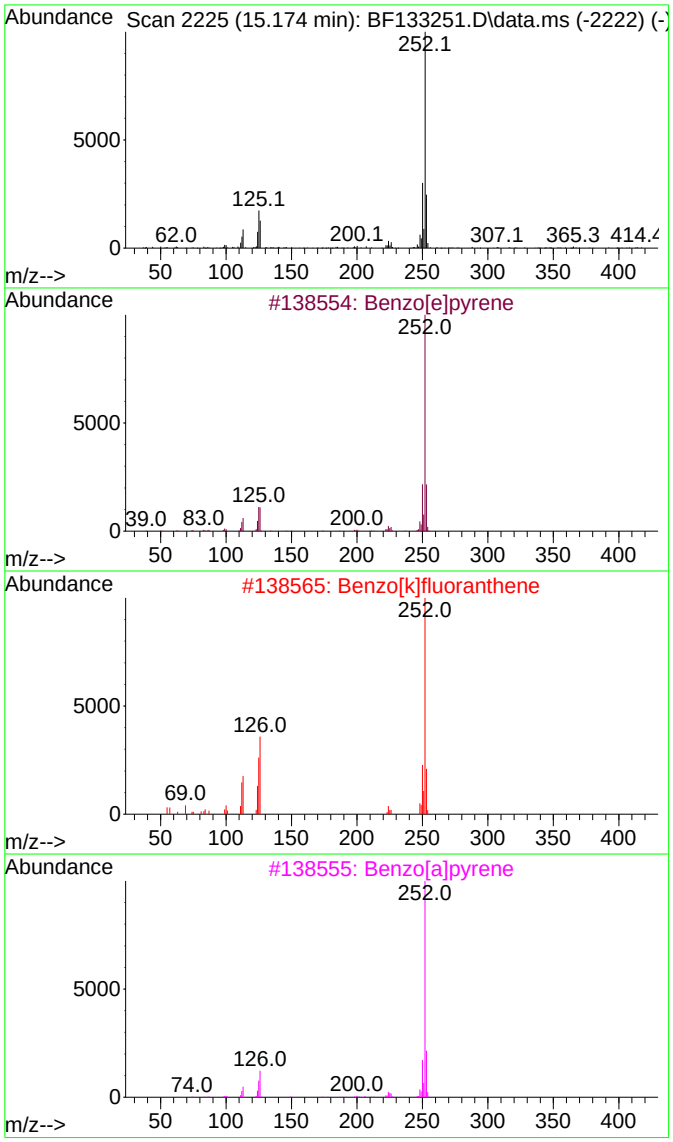
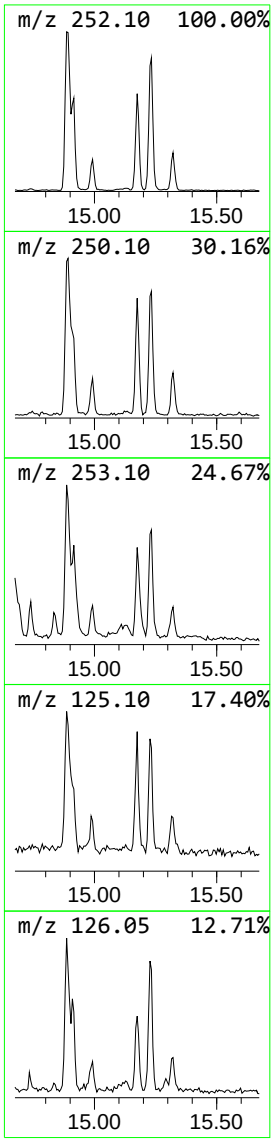
Peak Number 8 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	6.48 ng	261068	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3	Benzo[a]pyrene	252	C20H12	000050-32-8	96
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Perylene	252	C20H12	000198-55-0	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
Data File : BF133251.D
Acq On : 05 May 2023 01:44
Operator : CG\JU
Sample : 02588-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ZONE-B-0-3-05012023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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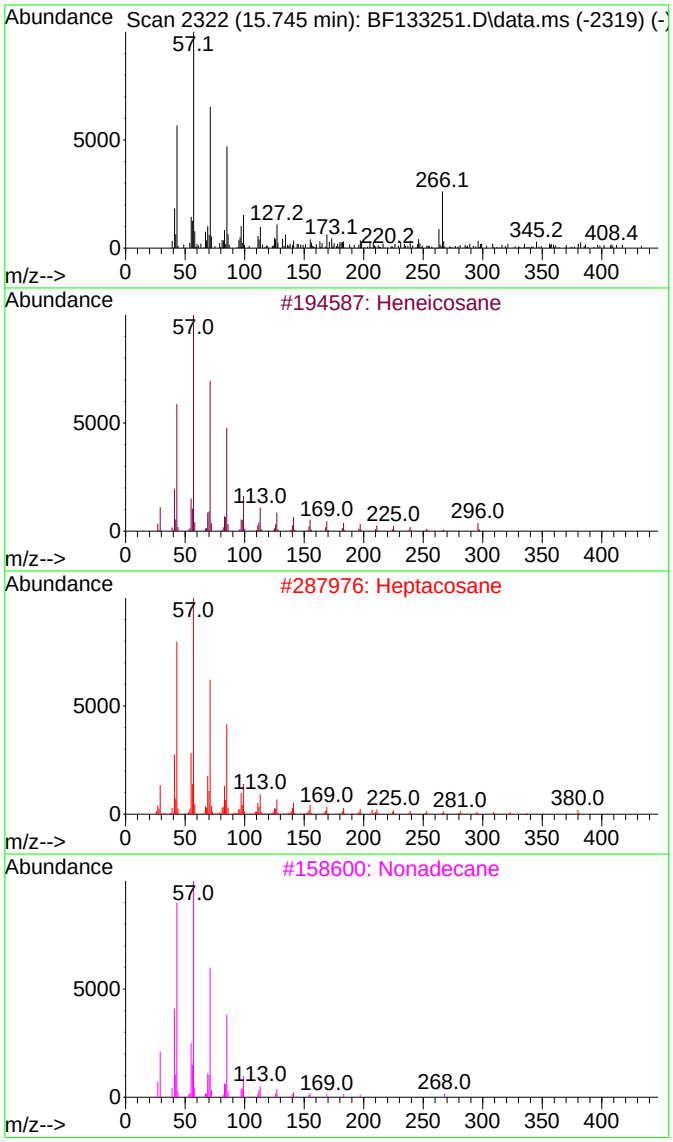
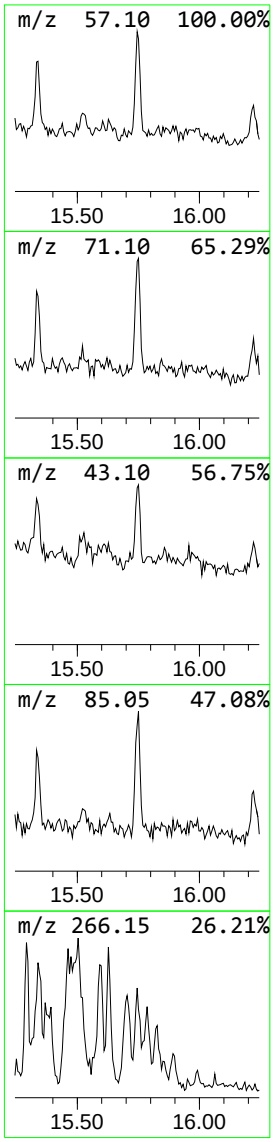
Peak Number 9 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.745	2.97 ng	119565	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	83
2	Heptacosane	380	C27H56	000593-49-7	70
3	Nonadecane	268	C19H40	000629-92-5	64
4	Decane, 1-iodo-	268	C10H21I	002050-77-3	64
5	Hexadecane	226	C16H34	000544-76-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
Data File : BF133251.D
Acq On : 05 May 2023 01:44
Operator : CG\JU
Sample : 02588-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ZONE-B-0-3-05012023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

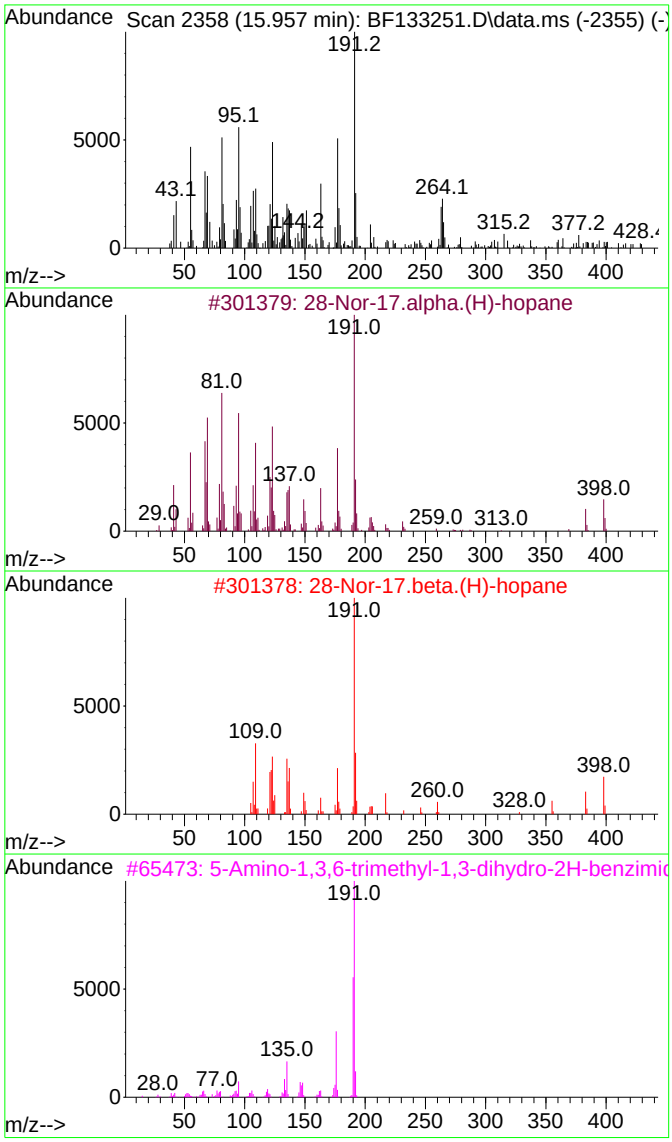
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

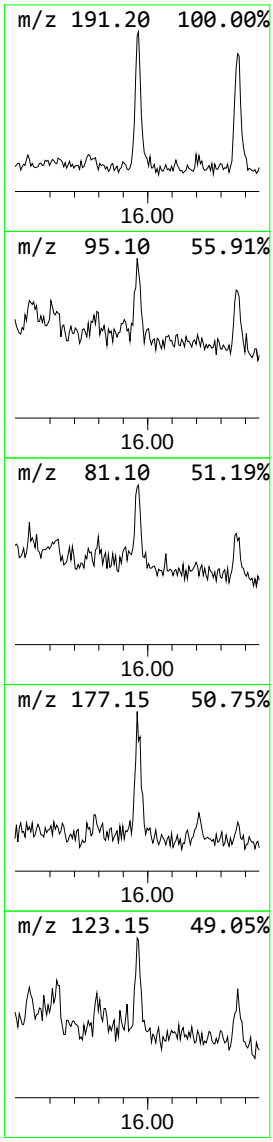
****

Peak Number 10 28-Nor-17.alpha.(H)-hopane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.957	6.80 ng	273765	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	86
2	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	46
3	5-Amino-1,3,6-trimethyl-1,3-dihy...	191	C10H13N3O	073778-94-6	27
4	(7S,7aR,13aS)-9-Methoxy-4,4,7,7a...	344	C22H32O3	1000482-45-3	27
5	A'-Neogammacer-22(29)-ene	410	C30H50	001615-91-4	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
Data File : BF133251.D
Acq On : 05 May 2023 01:44
Operator : CG\JU
Sample : 02588-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ZONE-B-0-3-05012023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
Benzophenone	10.469	3.5	ng	269638	3	9.757	1563070	20.0
n-Hexadecanoic ...	11.775	4.3	ng	296580	4	11.239	1362950	20.0
4H-Cyclopenta[d...	11.851	2.7	ng	185785	4	11.239	1362950	20.0
11H-Benzo[a]flu...	13.004	2.1	ng	158954	5	13.874	1504690	20.0
Pyrene, 1-methyl-	13.075	2.4	ng	178463	5	13.874	1504690	20.0
Nonadecane	13.739	3.0	ng	226245	5	13.874	1504690	20.0
Benzo[e]pyrene	15.174	6.5	ng	261068	6	15.292	805209	20.0
Heneicosane	15.745	3.0	ng	119565	6	15.292	805209	20.0
28-Nor-17.alpha...	15.957	6.8	ng	273765	6	15.292	805209	20.0