LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134737.D
Acq On : 11 Aug 2023 17:38
Operator : CG\JU
Sample : 03971-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-PP02A

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: BF134737.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	12	16	22	rVB	25670	35200	1.32%	0.131%
2	5.034	497	501	508	rVB	42969	52200	1.96%	0.194%
3	5.428	564	568	572	rBV	2726084	2495485	93.78%	9.286%
4	6.434	734	739	742	rBV	2619804	2389641	89.80%	8.892%
5	6.628	770	772	778	rBV	50062	56768	2.13%	0.211%
6	6.798	797	801	804	rBV	1472459	1121740	42.16%	4.174%
7	7.357	891	896	899	rBV	1784634	1532032	57.57%	5.701%
8	8.075	1014	1018	1022	rBV	1681732	1371194	51.53%	5.102%
9	9.151	1197	1201	1212	rBV	2987312	2660955	100.00%	9.901%
10	9.269	1218	1221	1225	rBV	38564	33679	1.27%	0.125%
11	9.834	1310	1317	1320	rBV	1350234	1275743	47.94%	4.747%
12	10.622	1446	1451	1460	rBV	1526795	1467990	55.17%	5.462%
13	11.322	1566	1570	1572	rBV	1342243	1210174	45.48%	4.503%
14	11.339	1572	1573	1577	rVV	185434	156747	5.89%	0.583%
15	11.392	1579	1582	1585	rVB	55004	52810	1.98%	0.197%
16	11.475	1593	1596	1599	rBV	65934	53999	2.03%	0.201%
17	11.551	1606	1609	1612	rBV	24846	30673	1.15%	0.114%
18	11.822	1652	1655	1657	rBV2	61454	55545	2.09%	0.207%
19	11.857	1657	1661	1665	rVV2	536950	487120	18.31%	1.813%
20	11.933	1671	1674	1677	rBV	75332	91170	3.43%	0.339%
21	11.957	1677	1678	1683	rVB	46531	31647	1.19%	0.118%
22	12.122	1703	1706	1708	rBV	31408	32058	1.20%	0.119%
23	12.139	1708	1709	1713	rVB2	30702	29838	1.12%	0.111%
24	12.269	1725	1731	1734	rBV5	29982	49051	1.84%	0.183%
25	12.375	1746	1749	1752	rBV	66320	66226	2.49%	0.246%
26	12.457	1761	1763	1768	rBV2	39825	51218	1.92%	0.191%
27	12.533	1773	1776	1780	rBV	634615	558121	20.97%	2.077%
28	12.645	1791	1795	1800	rBV3	160831	176662	6.64%	0.657%
29	12.763	1810	1815	1818	rBV	622951	609815	22.92%	2.269%
30	12.816	1822	1824	1829	rVB2	37475	47408	1.78%	0.176%
31	12.916	1837	1841	1844	rBV	3030196	2622948	98.57%	9.760%
32	12.986	1849	1853	1856	rBV2	63981	88312	3.32%	0.329%
33	13.069	1864	1867	1869	rBV4	44310	55060	2.07%	0.205%
34	13.092	1869	1871	1875	rVB	103926	90675	3.41%	0.337%
35	13.139	1876	1879	1880	rBV3	32957	35144	1.32%	0.131%
36	13.163	1880	1883	1885	rVB3	79101	76879	2.89%	0.286%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134737.D
Acq On : 11 Aug 2023 17:38
Operator : CG\JU
Sample : 03971-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-PP02A

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	13.198	1886	1889	1892	rBV2	90044	77373	2.91%	0.288%
38	13.292	1902	1905	1907	rVB	68074	52220	1.96%	0.194%
39	13.322	1907	1910	1912	rBV	67050	49567	1.86%	0.184%
40	13.351	1912	1915	1917	rBV3	35611	33415	1.26%	0.124%
41	13.498	1937	1940	1942	rBV2	46410	43500	1.63%	0.162%
42	13.616	1956	1960	1963	rVB2	48363	69621	2.62%	0.259%
43	13.716	1973	1977	1980	rBV3	73108	104677	3.93%	0.389%
44	13.745	1980	1982	1984	rVV	65037	56392	2.12%	0.210%
45	13.769	1984	1986	1991	rVV2	64520	91324	3.43%	0.340%
46	13.827	1992	1996	2003	rVB2	432450	514734	19.34%	1.915%
47	13.969	2015	2020	2023	rBV2	1319996	1629118	61.22%	6.062%
48	13.992	2023	2024	2030	rVB	352733	249493	9.38%	0.928%
49	14.074	2035	2038	2042	rVB	82439	68728	2.58%	0.256%
50	14.151	2048	2051	2054	rBV4	48304	51091	1.92%	0.190%
51	14.357	2084	2086	2089	rVB	67218	49967	1.88%	0.186%
52	14.469	2100	2105	2114	rVB3	198409	390264	14.67%	1.452%
53	14.839	2165	2168	2173	rVB2	100095	116621	4.38%	0.434%
54	14.910	2177	2180	2184	rVB2	117062	127053	4.77%	0.473%
55	15.010	2193	2197	2205	rVB	239190	451067	16.95%	1.678%
56	15.110	2211	2214	2217	rBV2	79219	96213	3.62%	0.358%
57	15.139	2217	2219	2226	rVB3	67051	88374	3.32%	0.329%
58	15.310	2245	2248	2254	rVB	158736	191570	7.20%	0.713%
59	15.374	2255	2259	2263	rBV	173643	221241	8.31%	0.823%
60	15.439	2266	2270	2273	rBV	620072	715448	26.89%	2.662%
61	15.945	2353	2356	2361	rVB2	59822	83837	3.15%	0.312%

Sum of corrected areas: 26874835

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Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134737.D
Acq On    : 11 Aug 2023  17:38
Operator  : CG\JU
Sample    : 03971-01
Misc      :
ALS Vial  : 9   Sample Multiplier: 1

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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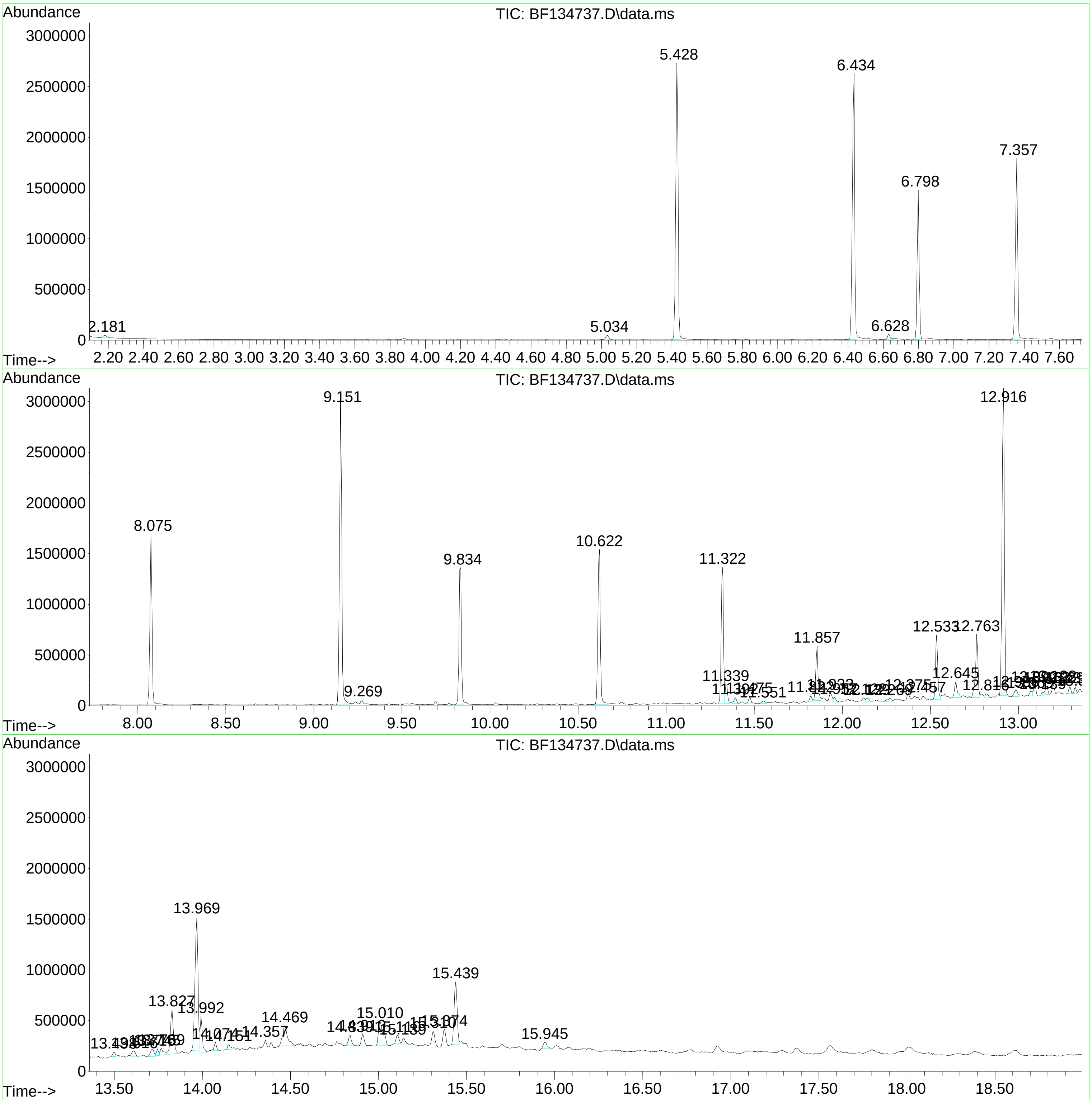
Instrument :
BNA_F
ClientSampleId :
B-PP02A



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Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
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Acq On    : 11 Aug 2023  17:38
Operator  : CG\JU
Sample    : 03971-01
Misc      :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title  : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

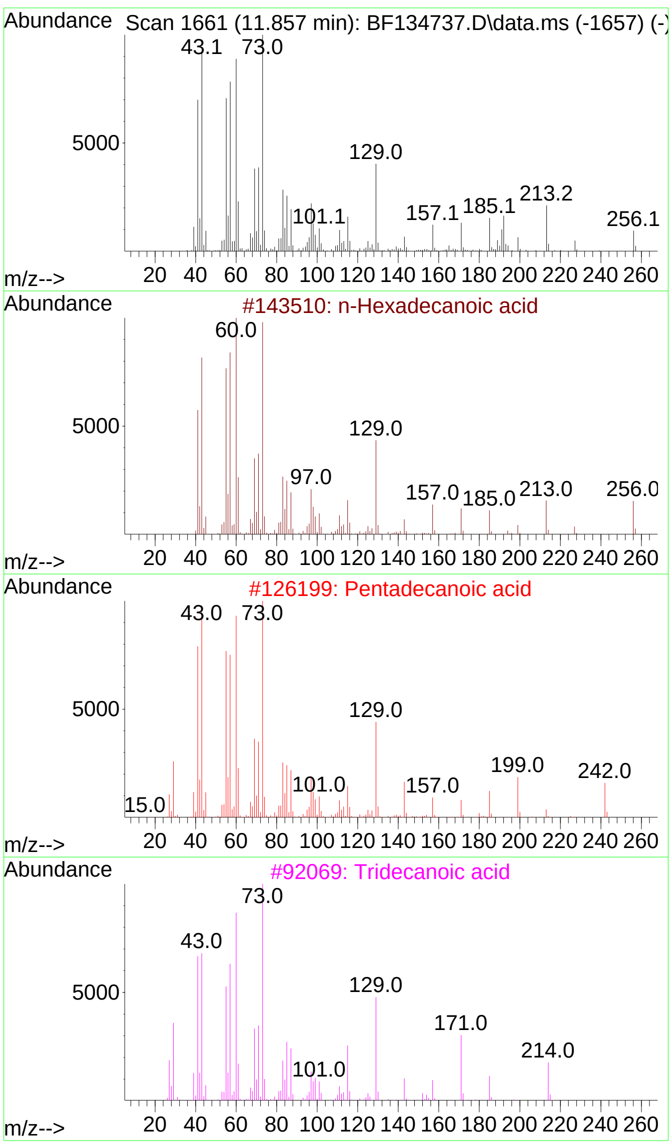
TIC Library    : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P
```

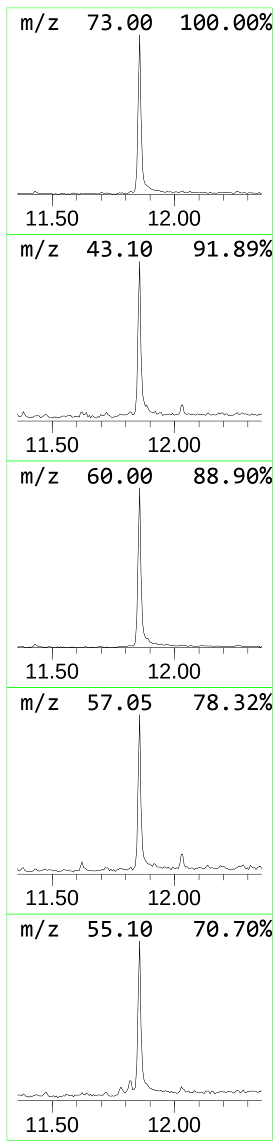
Instrument :
BNA_F
ClientSampleId :
B-PP02A

```
**********************************************************************
Peak Number  1  n-Hexadecanoic acid           Concentration Rank  1
```

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	8.05 ng	487120	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	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	92
4	Undecanoic acid	186	C11H22O2	000112-37-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134737.D
Acq On : 11 Aug 2023 17:38
Operator : CG\JU
Sample : 03971-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-PP02A

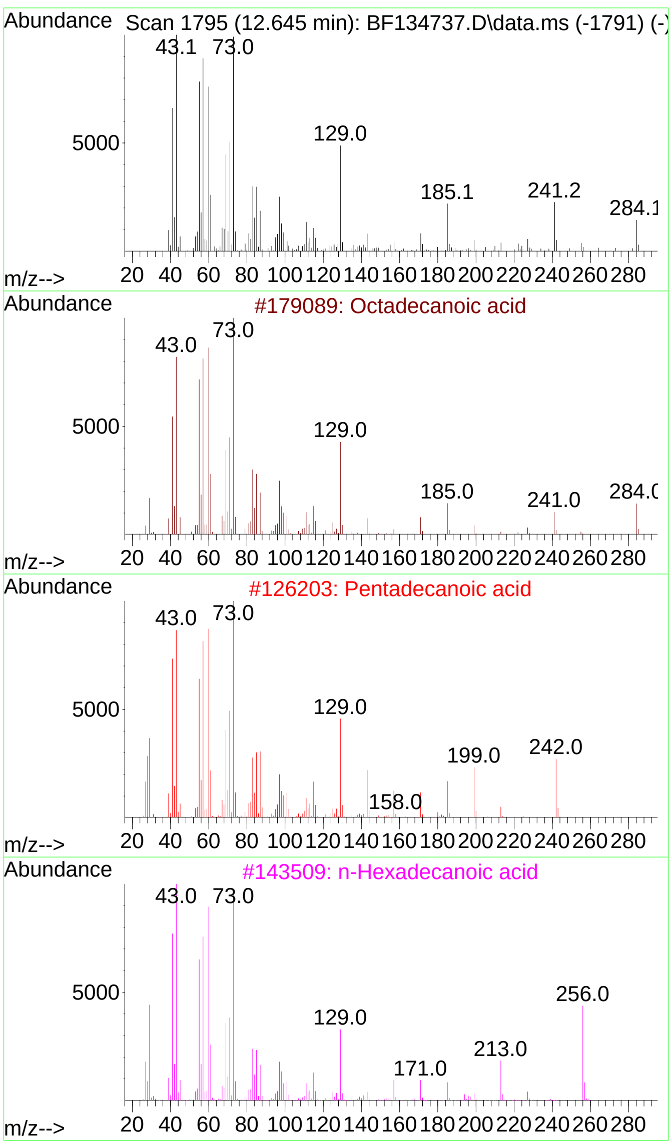
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

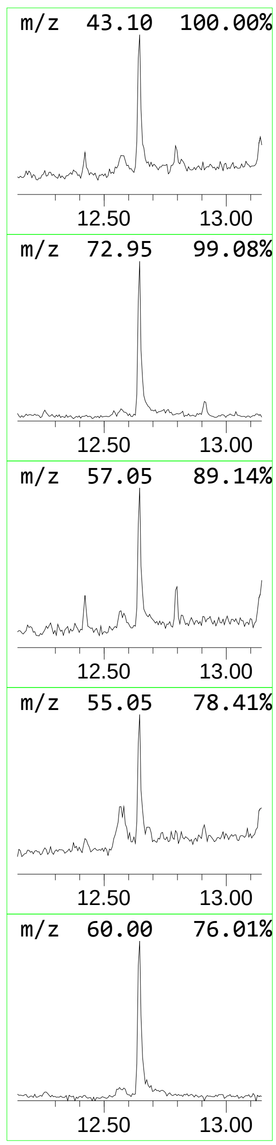
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	2.92 ng	176662	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	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134737.D
Acq On : 11 Aug 2023 17:38
Operator : CG\JU
Sample : 03971-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-PP02A

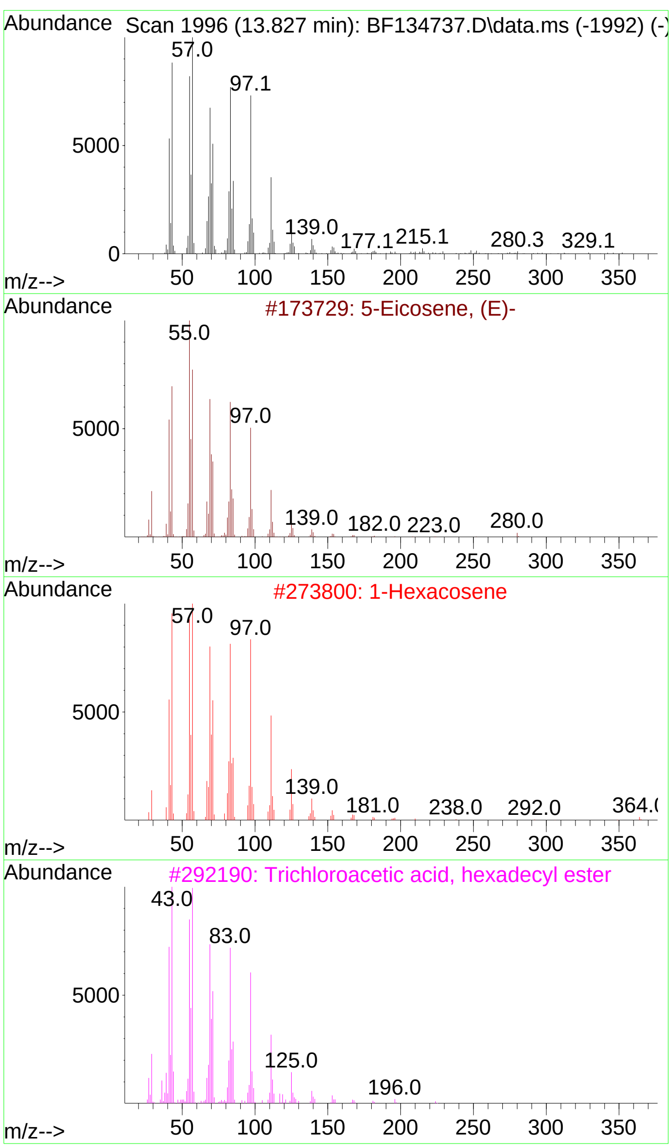
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

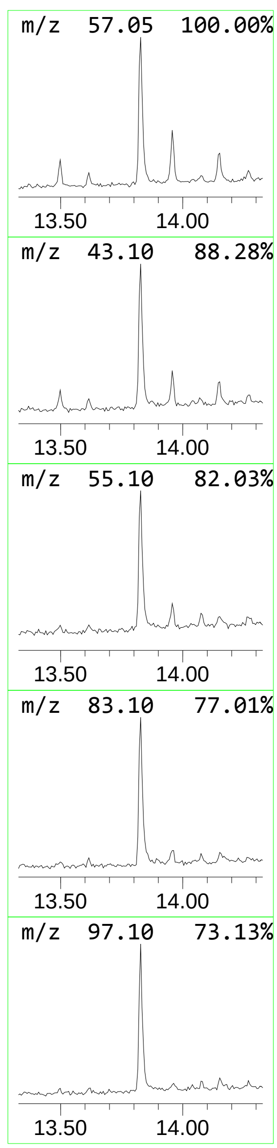
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	6.32 ng	514734	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	1-Hexacosene	364	C26H52	018835-33-1	95
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	Cyclotetracosane	336	C24H48	000297-03-0	94





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Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
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Acq On    : 11 Aug 2023  17:38
Operator  : CG\JU
Sample    : O3971-01
Misc      :
ALS Vial  : 9   Sample Multiplier: 1

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
```
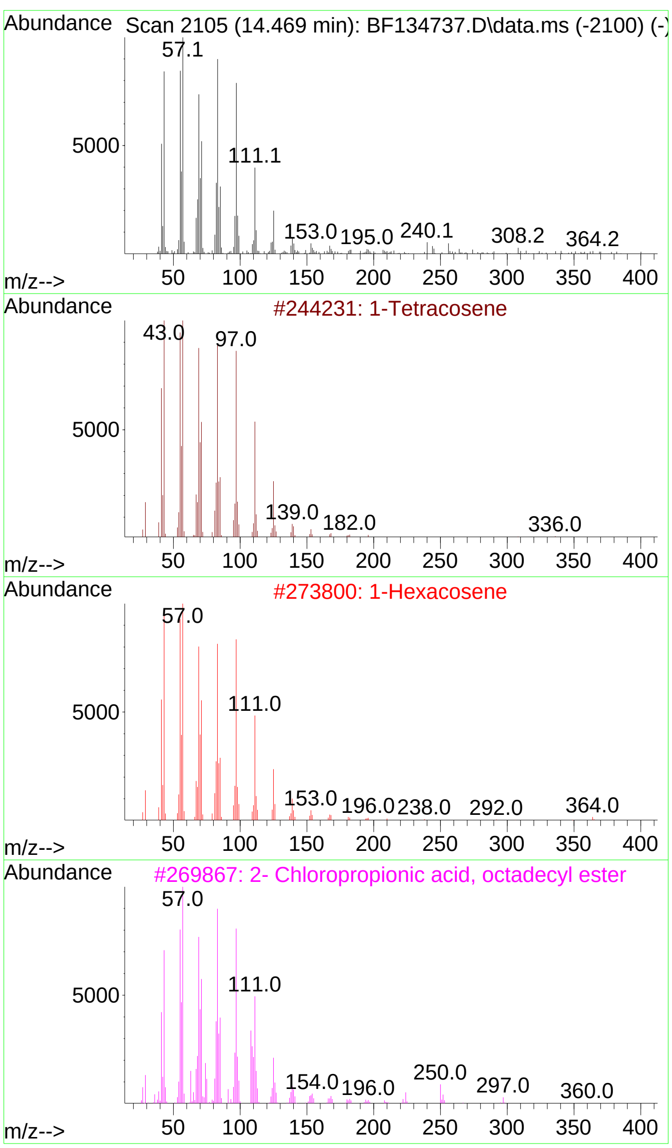
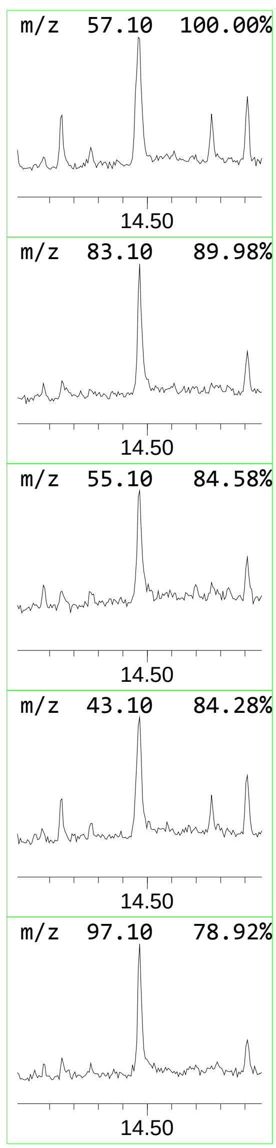

Instrument :
BNA_F
ClientSampleId :
B-PP02A

```
*********************************************************************
Peak Number  4  1-Tetracosene                   Concentration Rank  4
```

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.469	4.79 ng	390264	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	98
2	1-Hexacosene	364	C26H52	018835-33-1	97
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	96
4	Cyclotetracosane	336	C24H48	000297-03-0	96
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134737.D
Acq On : 11 Aug 2023 17:38
Operator : CG\JU
Sample : 03971-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-PP02A

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

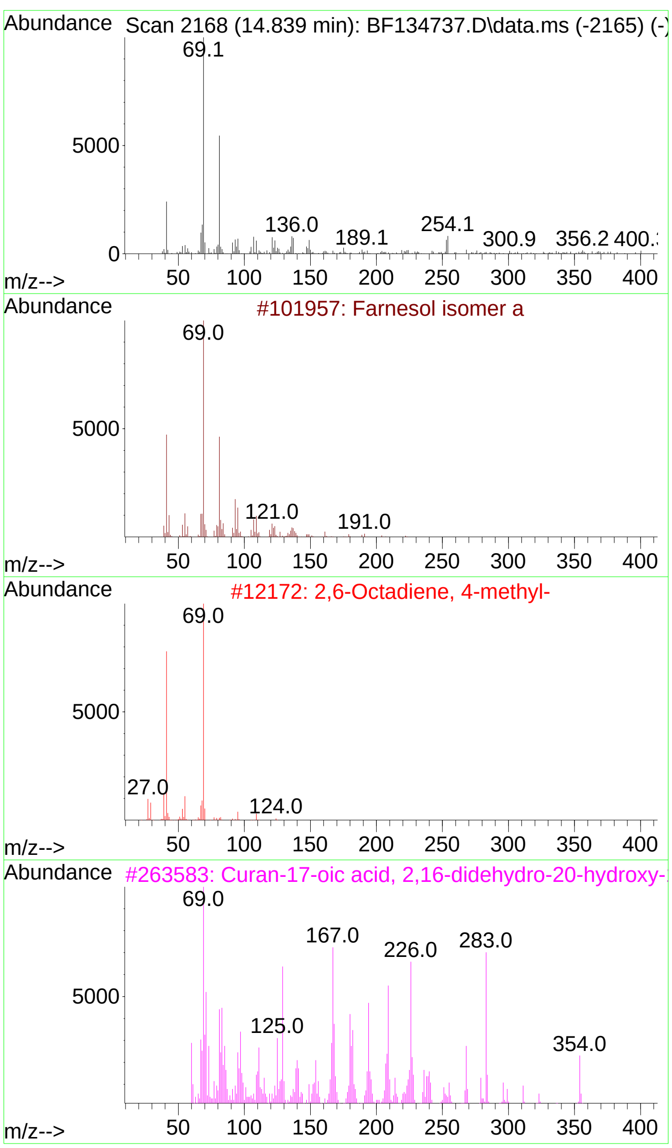
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

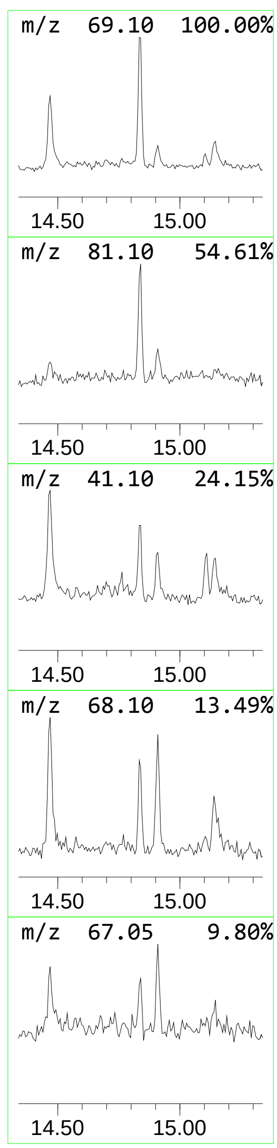
****

Peak Number 5 Farnesol isomer a Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	3.26 ng	116621	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Farnesol isomer a	222	C15H26O	1000108-92-4	76
2	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	64
3	Curan-17-oic acid, 2,16-didehydr...	354	C20H22N2O4	056053-15-7	64
4	2,6-Octadiene, 4,5-dimethyl-	138	C10H18	018476-57-8	59
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	59





Library Search Compound Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134737.D
Acq On : 11 Aug 2023 17:38
Operator : CG\JU
Sample : 03971-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-PP02A

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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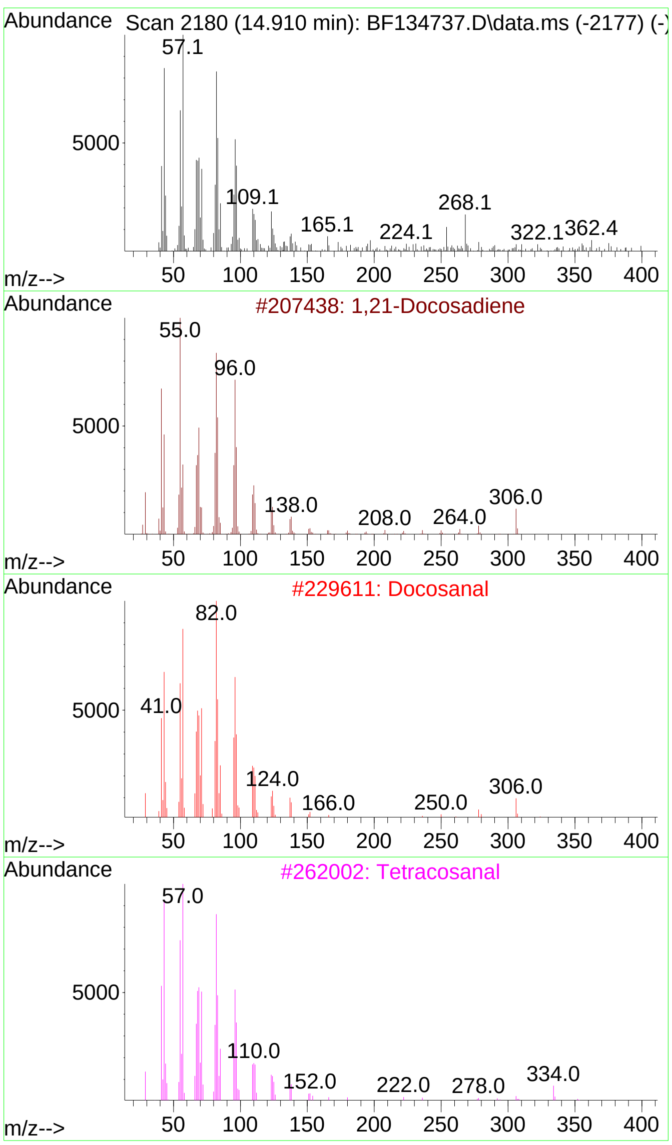
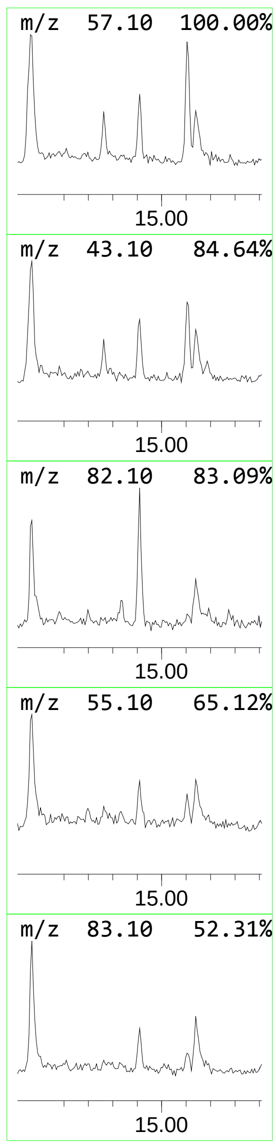
Peak Number 6 1,21-Docosadiene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.910	3.55 ng	127053	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,21-Docosadiene	306	C22H42	053057-53-7	97
2	Docosanal	324	C22H44O	057402-36-5	95
3	Tetracosanal	352	C24H48O	057866-08-7	95
4	1,19-Eicosadiene	278	C20H38	014811-95-1	93
5	Tetradecanal	212	C14H28O	000124-25-4	91





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Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134737.D
Acq On    : 11 Aug 2023  17:38
Operator  : CG\JU
Sample    : 03971-01
Misc      :
ALS Vial  : 9   Sample Multiplier: 1

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
```

Instrument :
BNA_F
ClientSampleId :
B-PP02A

```
**********************************************************************
Peak Number  7  Hexadecane                    Concentration Rank  8

  R.T.     EstConc          Area       Relative to ISTD         R.T.
----------------------------------------------------------------------
 15.110    2.69 ng          96213   Perylene-d12               15.439

 Hit# of  5    Tentative ID             MW  MolForm       CAS#       Qual
----------------------------------------------------------------------
 1 Benzo[b]fluoranthene                252 C20H12        000205-99-2 86
 2 Hexadecane                          226 C16H34        000544-76-3 70
 3 Benzo[a]pyrene                      252 C20H12        000050-32-8 59
 4 Heptadecane, 2,6,10,15-tetramethyl- 296 C21H44        054833-48-6 55
 5 Hexadecane, 2,6,10,14-tetramethyl-  282 C20H42        000638-36-8 49
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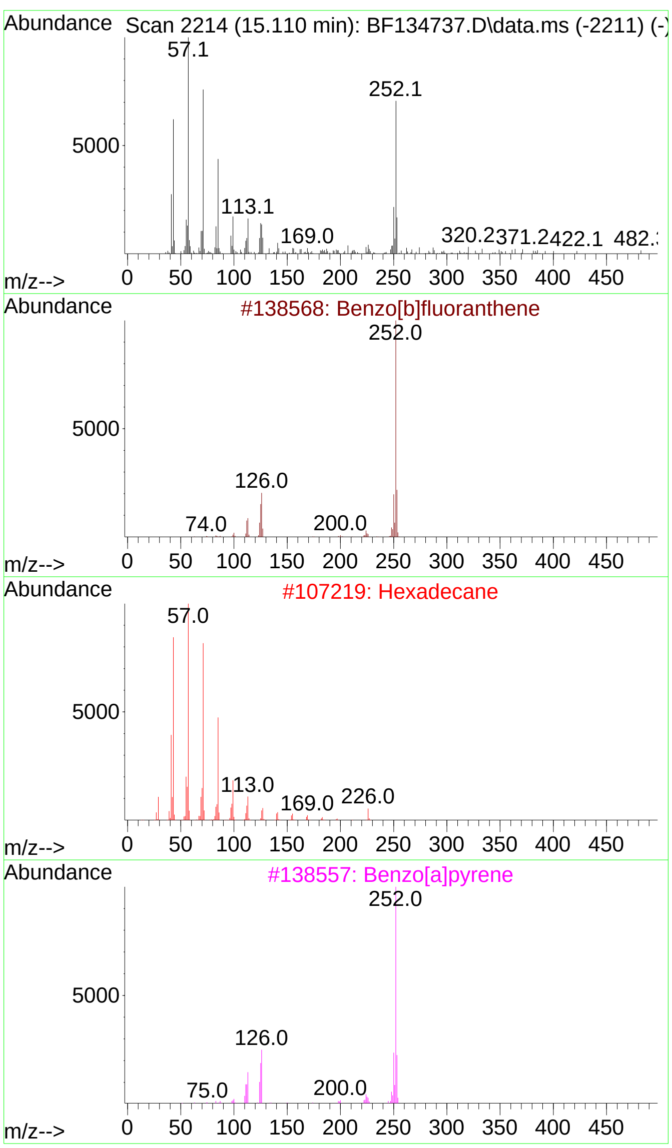
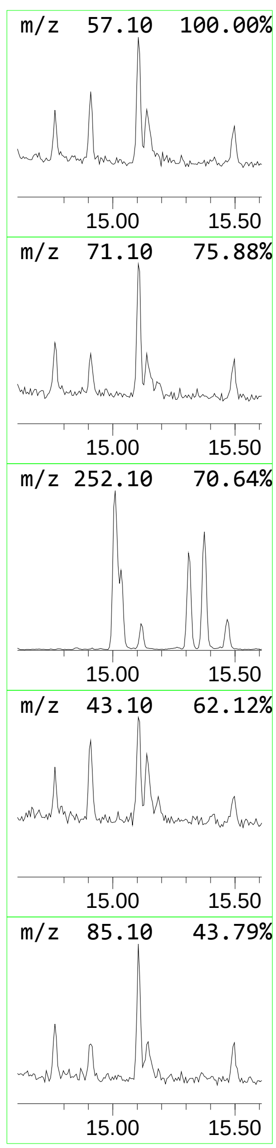




Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
Data File : BF134737.D
Acq On : 11 Aug 2023 17:38
Operator : CG\JU
Sample : 03971-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-PP02A

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

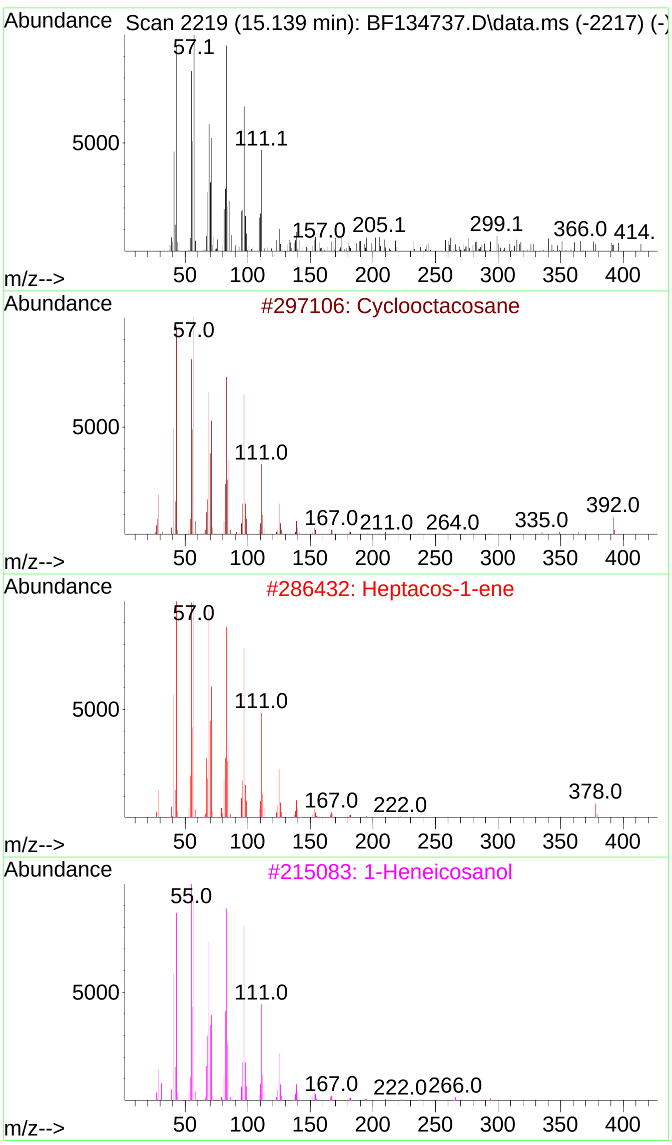
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

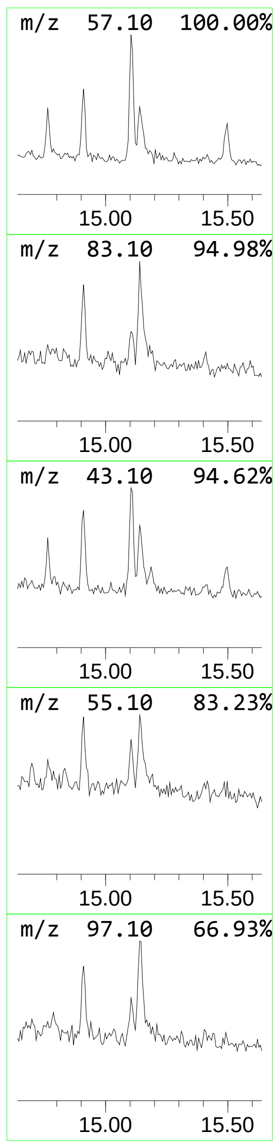
****

Peak Number 8 Cyclooctacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.139	2.47 ng	88374	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctacosane	392	C28H56	000297-24-5	87
2	Heptacos-1-ene	378	C27H54	015306-27-1	87
3	1-Heneicosanol	312	C21H44O	015594-90-8	87
4	Henicos-1-ene	294	C21H42	001599-68-4	83
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	68





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Operator : CG\JU
Sample : 03971-01
Misc :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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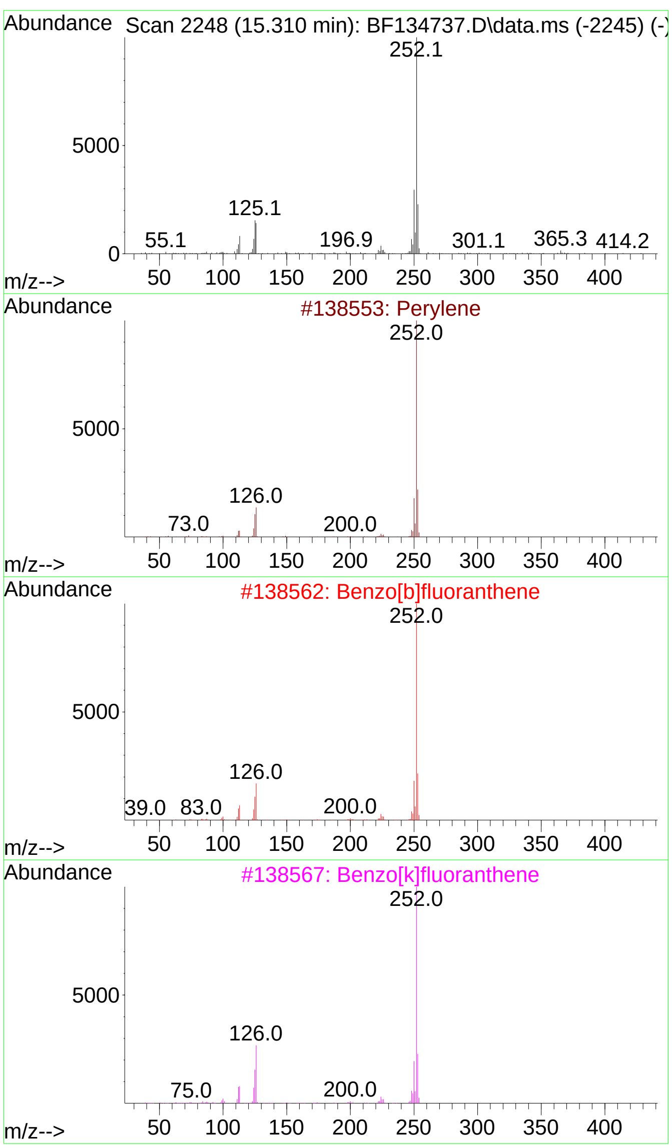
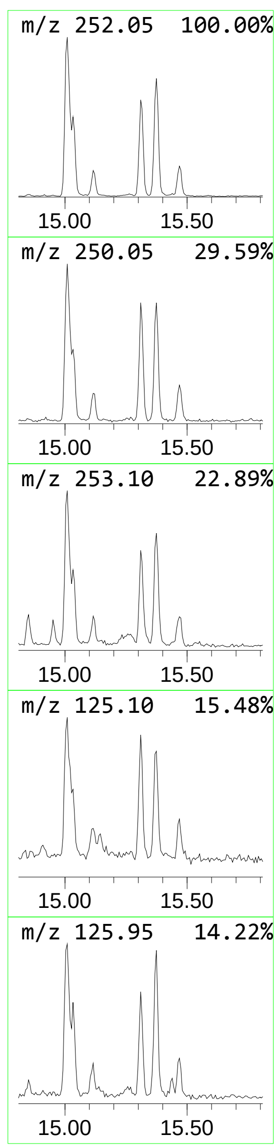
Peak Number 9 Perylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.310	5.36 ng	191570	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	96
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
5	Benzo[e]pyrene	252	C20H12	000192-97-2	94





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Operator : CG\JU
Sample : 03971-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-PP02A

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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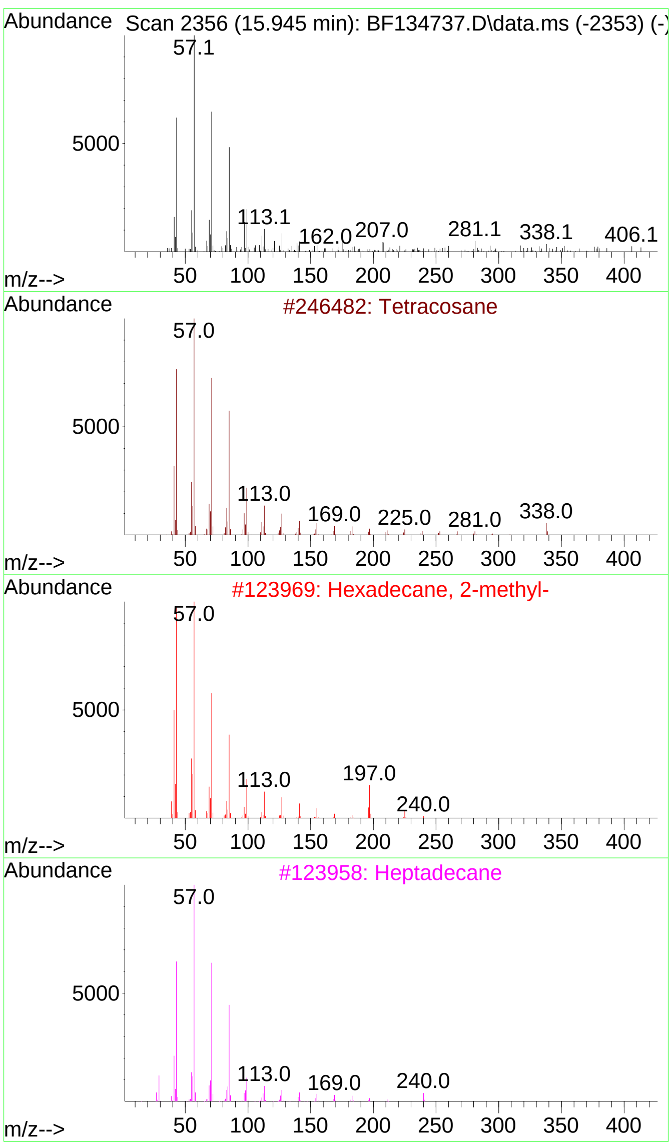
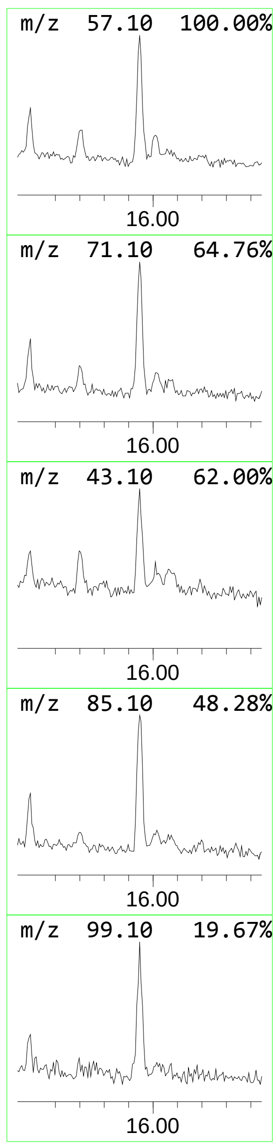
Peak Number 10 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	2.34 ng	83837	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	81
3	Heptadecane	240	C17H36	000629-78-7	76
4	Pentacosane	352	C25H52	000629-99-2	74
5	3,5-Dimethyldodecane	198	C14H30	107770-99-0	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
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Operator : CG\JU
Sample : O3971-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-PP02A

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
n-Hexadecanoic ...	11.857	8.1	ng	487120	4	11.322	1210170	20.0
Octadecanoic acid	12.645	2.9	ng	176662	4	11.322	1210170	20.0
5-Eicosene, (E)-	13.827	6.3	ng	514734	5	13.969	1629120	20.0
1-Tetracosene	14.469	4.8	ng	390264	5	13.969	1629120	20.0
Farnesol isomer a	14.839	3.3	ng	116621	6	15.439	715448	20.0
1,21-Docosadiene	14.910	3.5	ng	127053	6	15.439	715448	20.0
Hexadecane	15.110	2.7	ng	96213	6	15.439	715448	20.0
Cyclooctacosane	15.139	2.5	ng	88374	6	15.439	715448	20.0
Perylene	15.310	5.4	ng	191570	6	15.439	715448	20.0
Tetracosane	15.945	2.3	ng	83837	6	15.439	715448	20.0