LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051223\
Data File : BF133374.D
Acq On : 12 May 2023 17:45
Operator : CG\JU
Sample : 02747-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-0-2-20230510

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: BF133374.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.898	474	478	485	rVB	149855	172019	6.01%	0.600%
2	5.328	548	551	563	rBV	2605139	2647872	92.47%	9.243%
3	6.363	723	727	735	rBV	3024982	2680835	93.62%	9.358%
4	6.722	784	788	791	rBV	1348112	1089514	38.05%	3.803%
5	7.281	878	883	887	rBV	1773828	1659222	57.94%	5.792%
6	8.004	1003	1006	1009	rBV	1798257	1370071	47.85%	4.782%
7	8.716	1124	1127	1135	rBV2	40479	72828	2.54%	0.254%
8	9.080	1185	1189	1192	rBV	3777033	2863447	100.00%	9.995%
9	9.198	1206	1209	1212	rVB3	73458	61319	2.14%	0.214%
10	9.416	1243	1246	1249	rBV	262720	202790	7.08%	0.708%
11	9.463	1249	1254	1256	rBV3	38874	44868	1.57%	0.157%
12	9.616	1275	1280	1284	rVB2	103556	112537	3.93%	0.393%
13	9.657	1284	1287	1292	rBV4	34465	49275	1.72%	0.172%
14	9.757	1296	1304	1307	rBV	1794698	1642327	57.35%	5.733%
15	9.963	1334	1339	1343	rBV2	33715	45934	1.60%	0.160%
16	10.469	1421	1425	1428	rBV	139590	120857	4.22%	0.422%
17	10.545	1434	1438	1443	rBV	1554081	1323663	46.23%	4.620%
18	10.627	1448	1452	1456	rVV2	58167	66558	2.32%	0.232%
19	10.669	1456	1459	1467	rVB3	36272	59787	2.09%	0.209%
20	10.910	1497	1500	1507	rBV9	29591	54157	1.89%	0.189%
21	10.969	1507	1510	1514	rBV4	21853	39039	1.36%	0.136%
22	11.239	1552	1556	1558	rBV	1462394	1178805	41.17%	4.115%
23	11.263	1558	1560	1564	rVV	451859	342076	11.95%	1.194%
24	11.310	1564	1568	1572	rVB	73264	89814	3.14%	0.314%
25	11.469	1590	1595	1599	rBV2	55699	97678	3.41%	0.341%
26	11.739	1639	1641	1644	rBV	86807	74793	2.61%	0.261%
27	11.774	1644	1647	1651	rBV2	615185	649446	22.68%	2.267%
28	11.851	1657	1660	1663	rBV	72219	63742	2.23%	0.222%
29	12.063	1694	1696	1699	rVB	104829	80028	2.79%	0.279%
30	12.292	1732	1735	1739	rBV2	53264	81171	2.83%	0.283%
31	12.374	1746	1749	1752	rBV2	89408	98245	3.43%	0.343%
32	12.451	1757	1762	1765	rBV	763602	745118	26.02%	2.601%
33	12.486	1765	1768	1776	rVV6	178180	355649	12.42%	1.241%
34	12.563	1778	1781	1791	rVB3	184269	287716	10.05%	1.004%
35	12.680	1796	1801	1804	rVV	584447	595057	20.78%	2.077%
36	12.710	1804	1806	1813	rVB3	157881	229647	8.02%	0.802%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051223\
Data File : BF133374.D
Acq On : 12 May 2023 17:45
Operator : CG\JU
Sample : 02747-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-0-2-20230510

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	12.827	1822	1826	1829	rBV	2458211	2274655	79.44%	7.940%
38	13.063	1864	1866	1870	rVB2	78963	83740	2.92%	0.292%
39	13.198	1887	1889	1893	rBV	71429	69342	2.42%	0.242%
40	13.404	1922	1924	1927	rVB	122343	102351	3.57%	0.357%
41	13.733	1977	1980	1987	rVB2	346191	416823	14.56%	1.455%
42	13.874	1999	2004	2007	rBV2	1111249	1361491	47.55%	4.752%
43	14.051	2031	2034	2037	rVB	218795	181287	6.33%	0.633%
44	14.357	2084	2086	2088	rVB	203671	146254	5.11%	0.511%
45	14.892	2175	2177	2181	rBV	187330	225268	7.87%	0.786%
46	14.974	2188	2191	2194	rBV	609879	584197	20.40%	2.039%
47	15.298	2243	2246	2249	rBV	535356	585328	20.44%	2.043%
48	15.745	2318	2322	2327	rVB	954230	1269512	44.34%	4.431%

Sum of corrected areas: 28648152

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051223\
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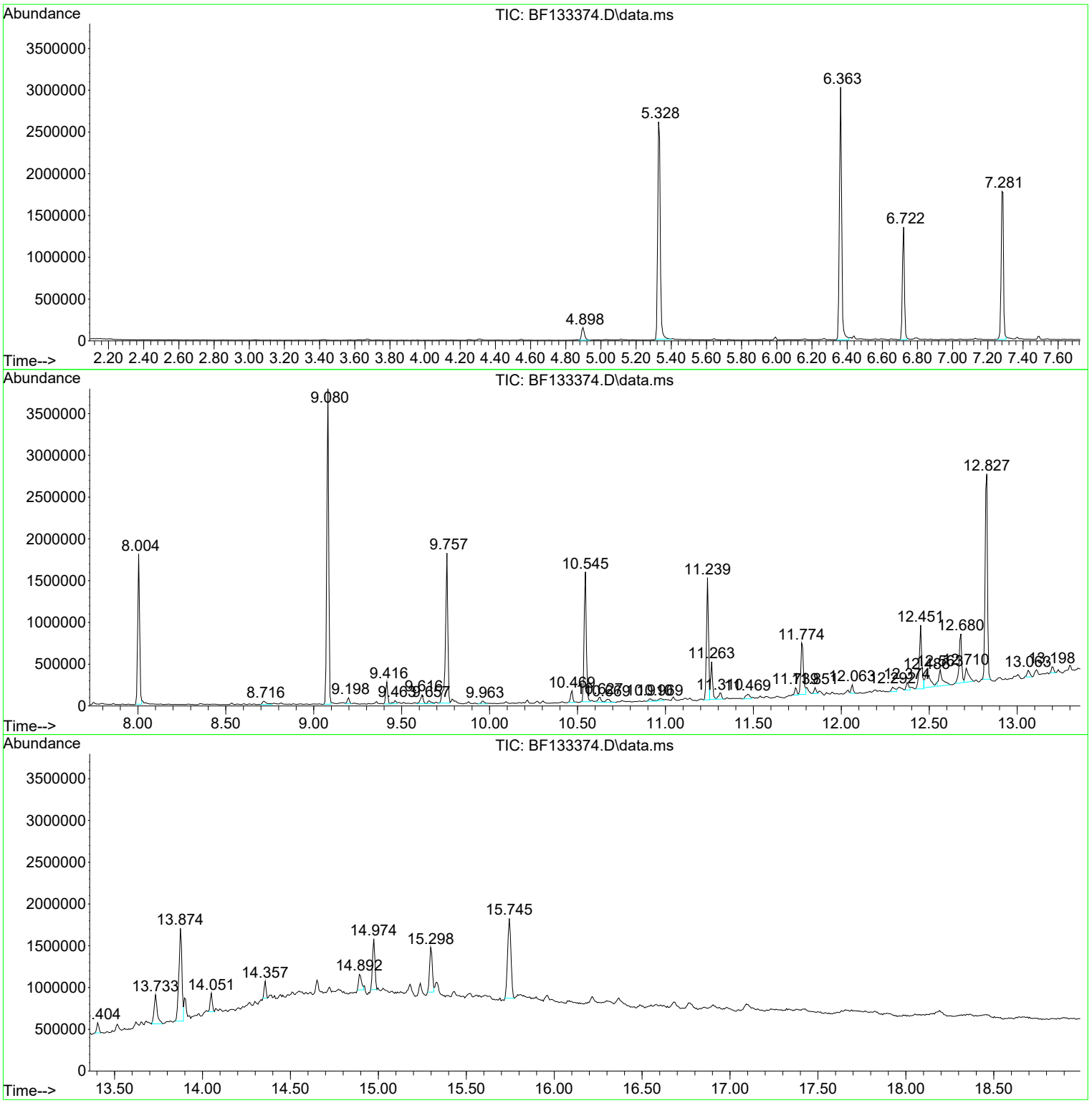
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-0-2-20230510

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\BF051223\
Data File : BF133374.D
Acq On : 12 May 2023 17:45
Operator : CG\JU
Sample : 02747-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-0-2-20230510

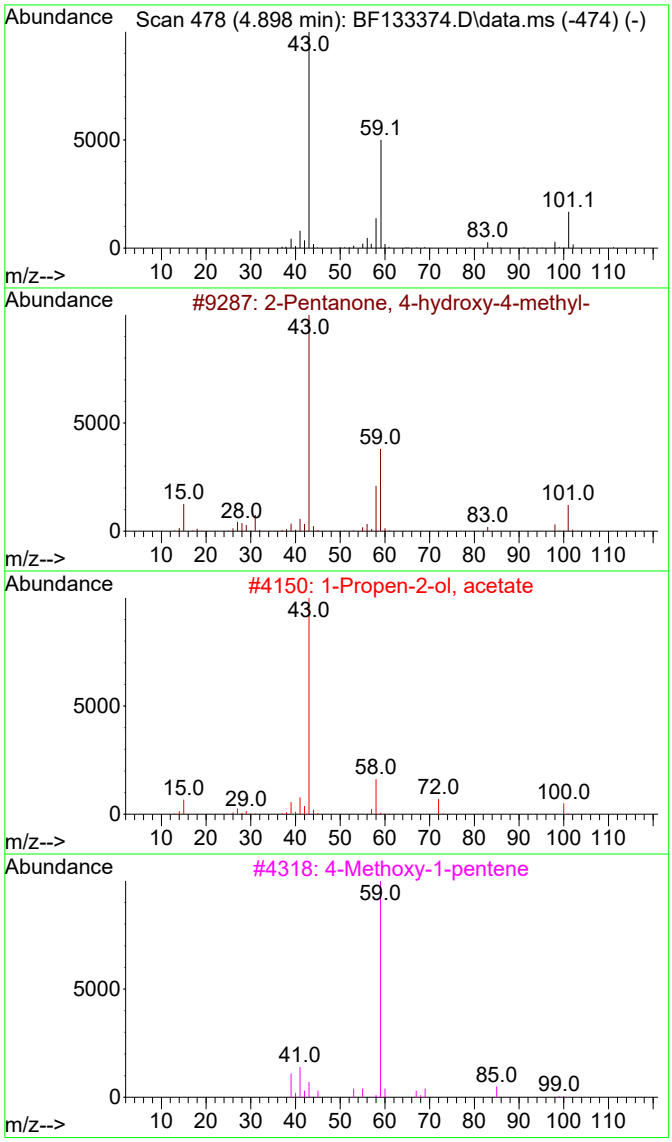
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

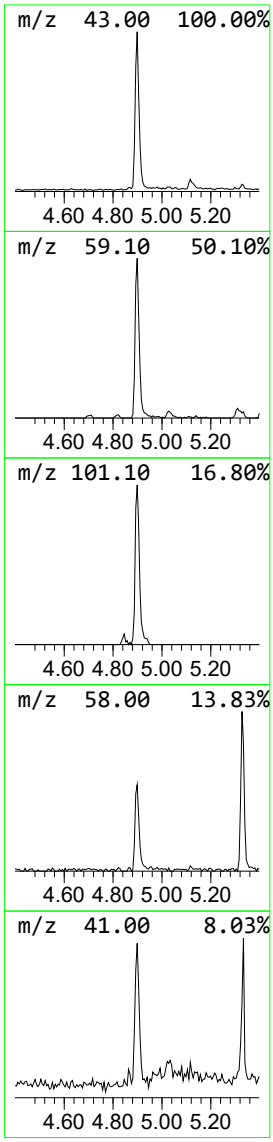
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.898	3.16 ng	172019	1,4-Dichlorobenzene-d4	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	9
4	Allyl acetate	100	C5H8O2	000591-87-7	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051223\
Data File : BF133374.D
Acq On : 12 May 2023 17:45
Operator : CG\JU
Sample : 02747-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-0-2-20230510

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

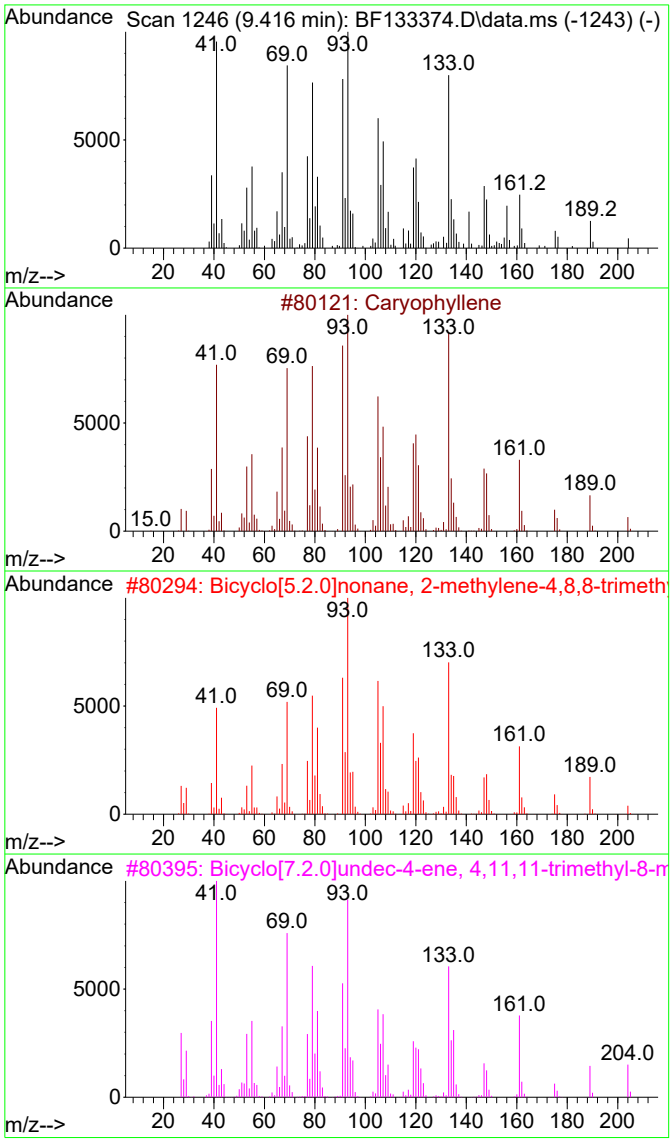
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

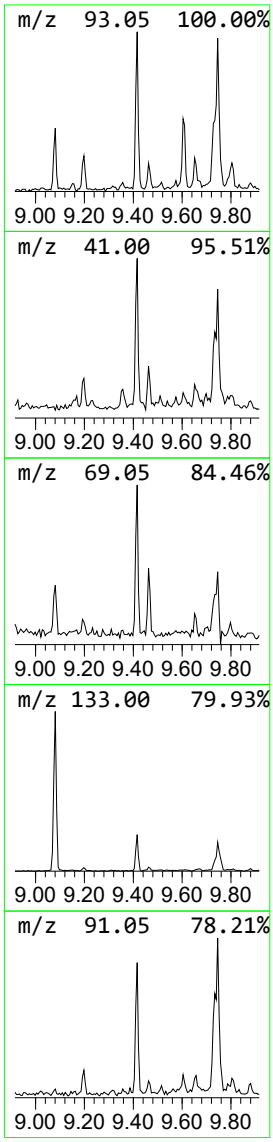
****

Peak Number 2 Caryophyllene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.416	2.47 ng	202790	Acenaphthene-d10	9.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caryophyllene	204	C15H24	000087-44-5	99
2	Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	95
3	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	90
4	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	89
5	.alpha.-Farnesene	204	C15H24	000502-61-4	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051223\
Data File : BF133374.D
Acq On : 12 May 2023 17:45
Operator : CG\JU
Sample : 02747-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-0-2-20230510

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

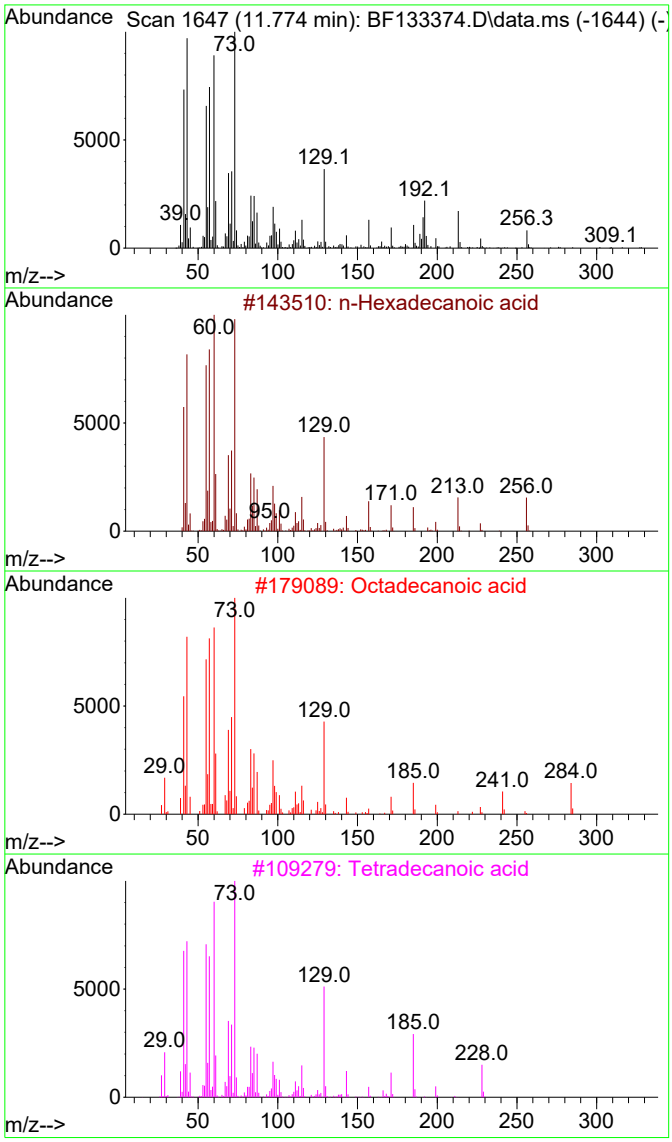
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

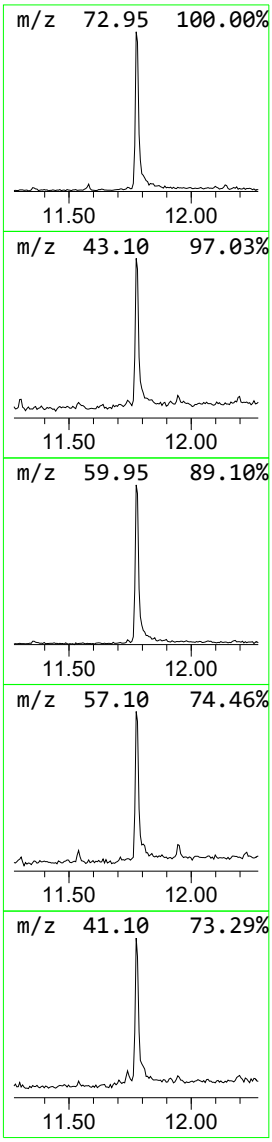
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.774	11.02 ng	649446	Phenanthrene-d10	11.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051223\
Data File : BF133374.D
Acq On : 12 May 2023 17:45
Operator : CG\JU
Sample : 02747-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-0-2-20230510

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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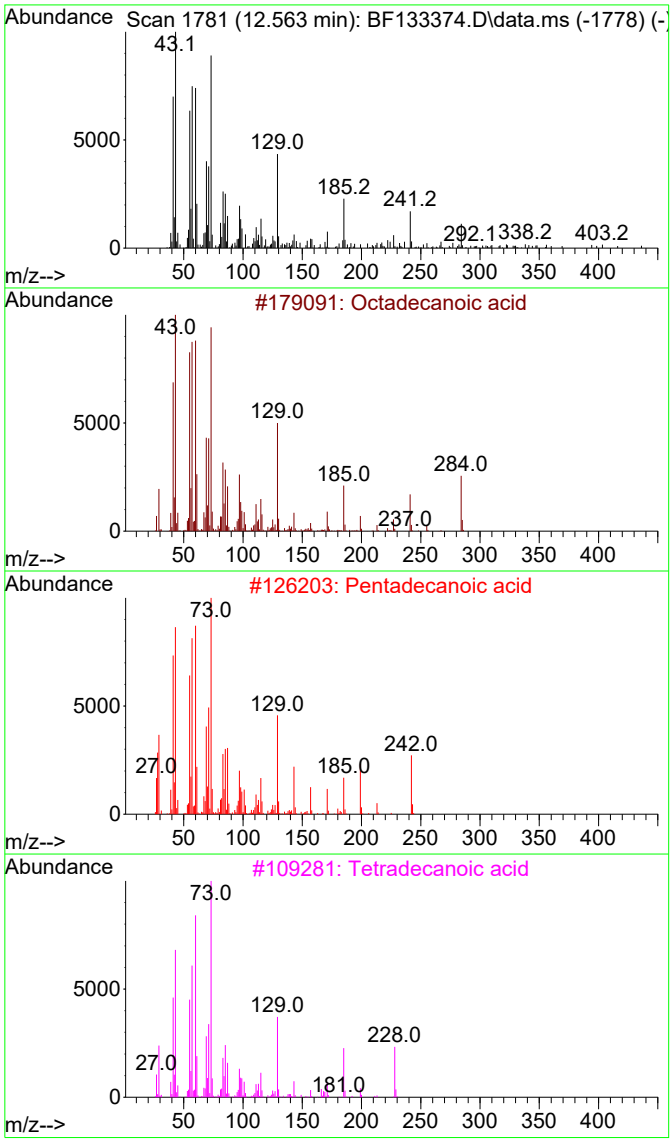
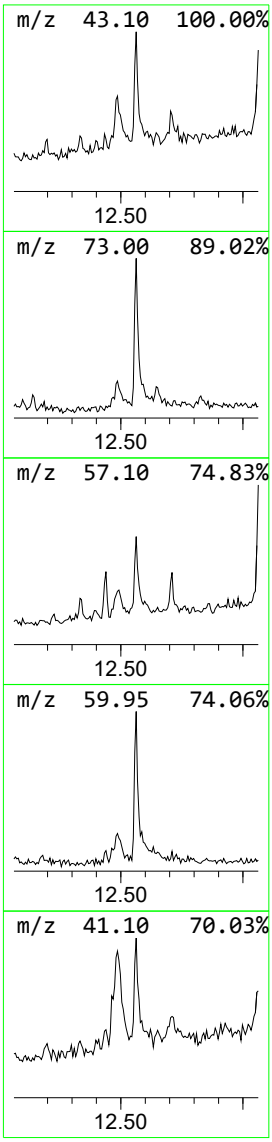
Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.563	4.23 ng	287716	Chrysene-d12	13.874

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	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051223\
Data File : BF133374.D
Acq On : 12 May 2023 17:45
Operator : CG\JU
Sample : 02747-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-0-2-20230510

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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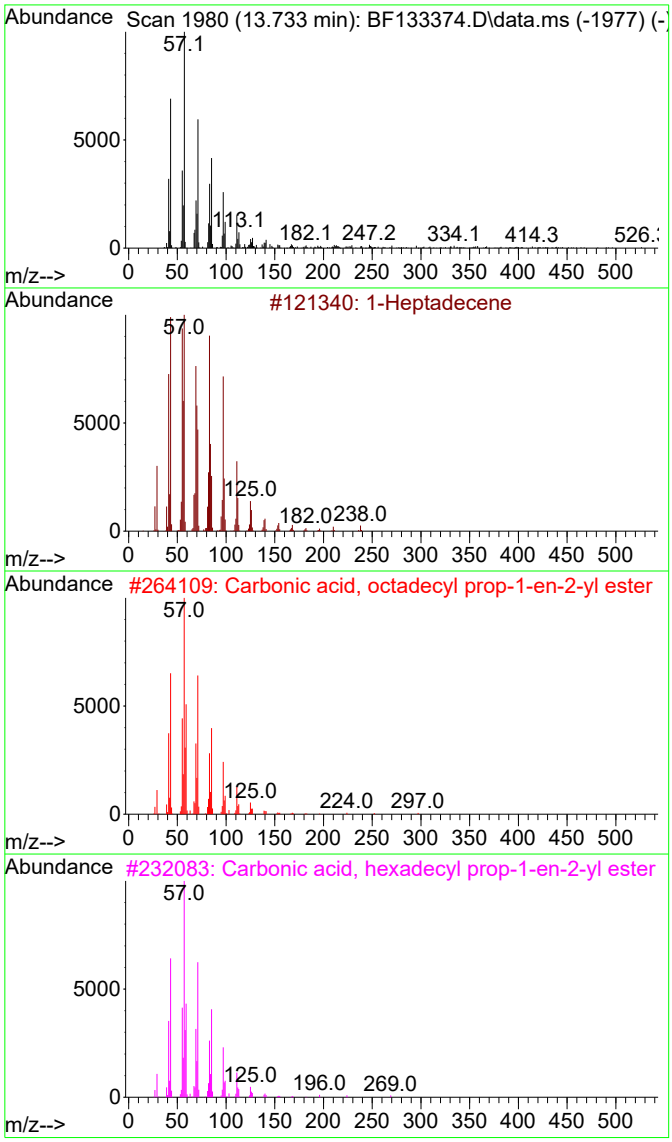
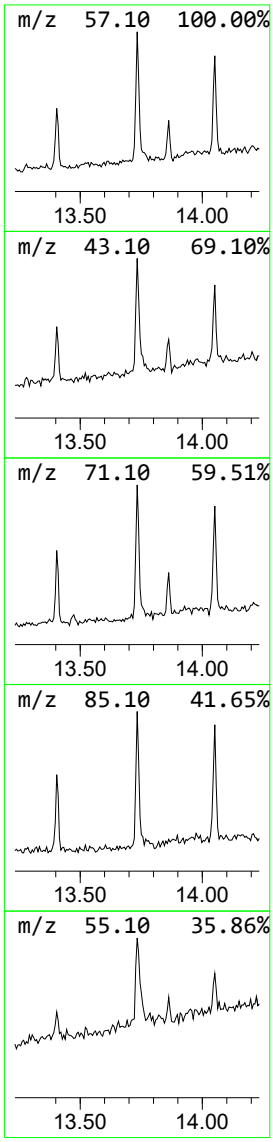
Peak Number 5 1-Heptadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.733	6.12 ng	416823	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptadecene	238	C17H34	006765-39-5	96
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	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	90
5	Carbonic acid, decyl hexadecyl e...	426	C27H54O3	1000383-16-5	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051223\
Data File : BF133374.D
Acq On : 12 May 2023 17:45
Operator : CG\JU
Sample : 02747-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-0-2-20230510

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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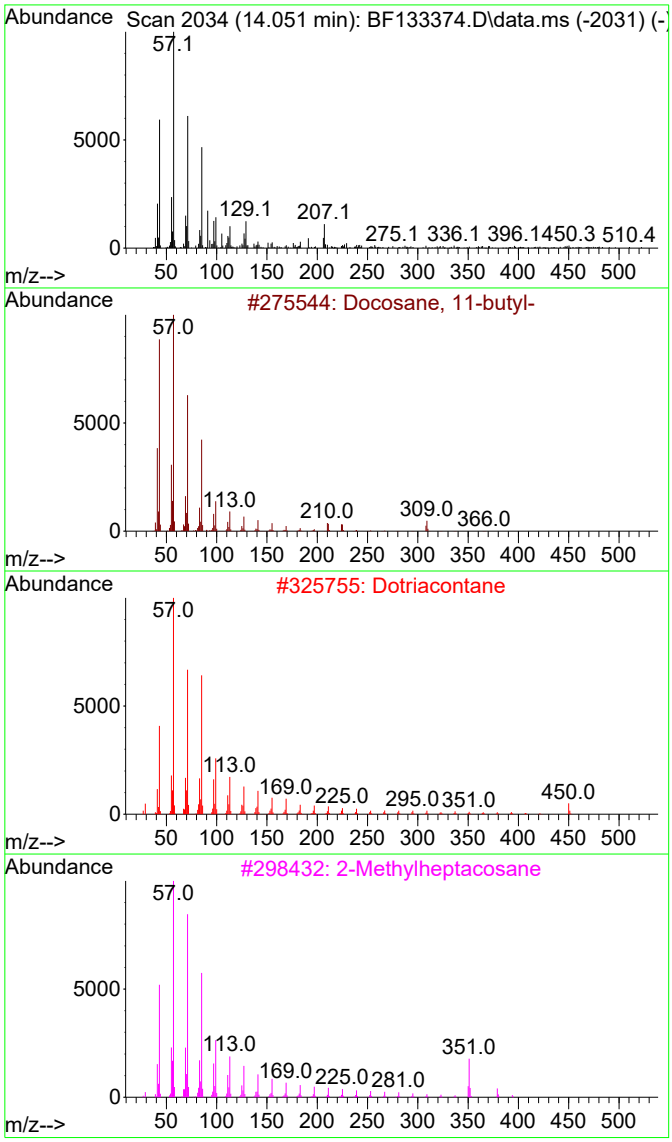
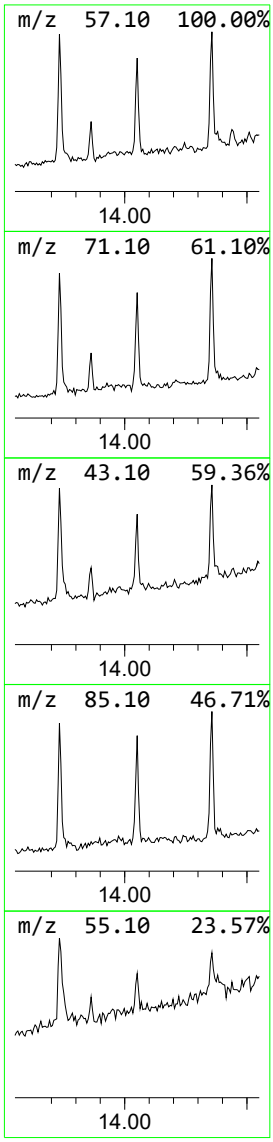
Peak Number 6 Docosane, 11-butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.051	2.66 ng	181287	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-	366	C26H54	013475-76-8	86
2	Dotriacontane	451	C32H66	000544-85-4	70
3	2-Methylheptacosane	394	C28H58	001561-00-8	70
4	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	70
5	Hexacosane	366	C26H54	000630-01-3	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051223\
Data File : BF133374.D
Acq On : 12 May 2023 17:45
Operator : CG\JU
Sample : 02747-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-0-2-20230510

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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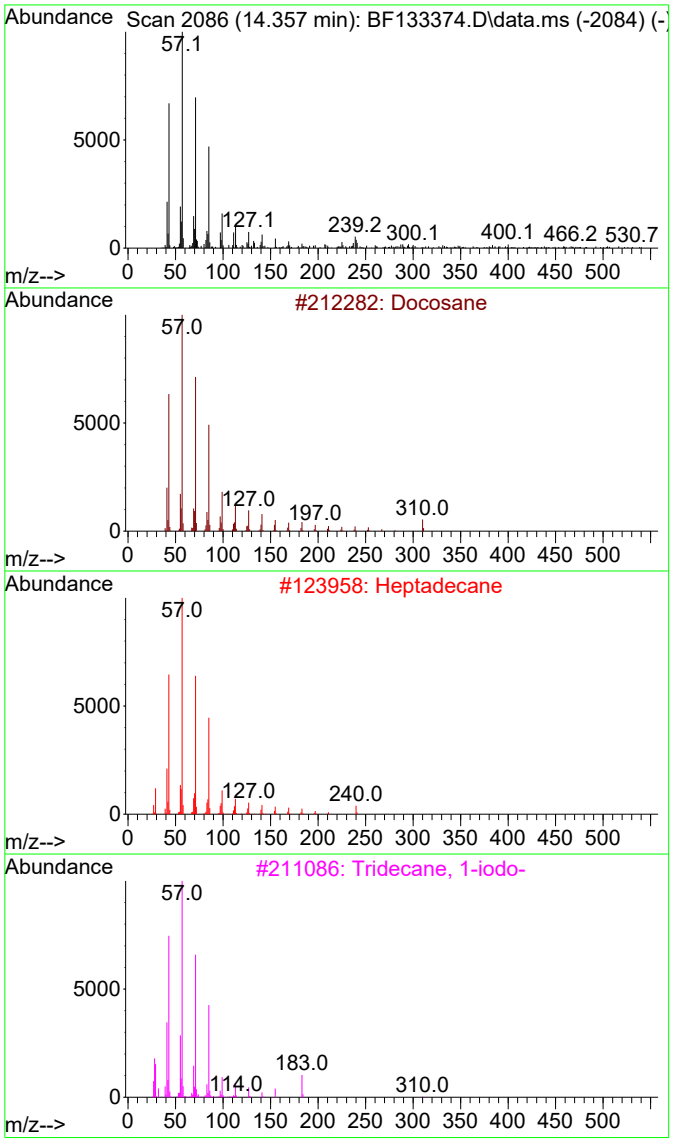
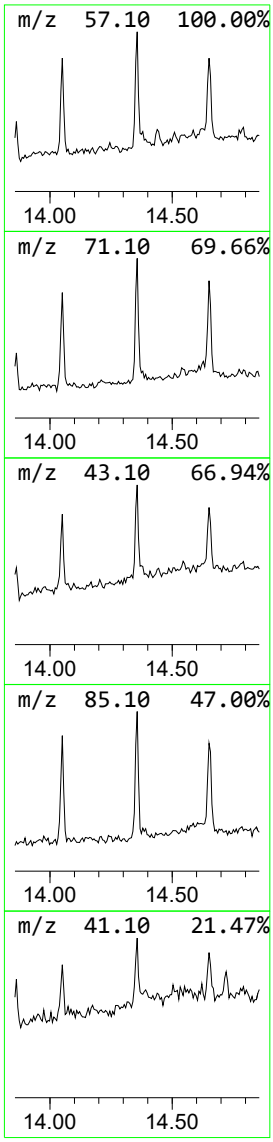
Peak Number 7 Docosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.357	2.15 ng	146254	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	97
2	Heptadecane	240	C17H36	000629-78-7	96
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	93
4	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	90
5	Dotriacontane, 2-methyl-	465	C33H68	001720-11-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051223\
Data File : BF133374.D
Acq On : 12 May 2023 17:45
Operator : CG\JU
Sample : 02747-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-0-2-20230510

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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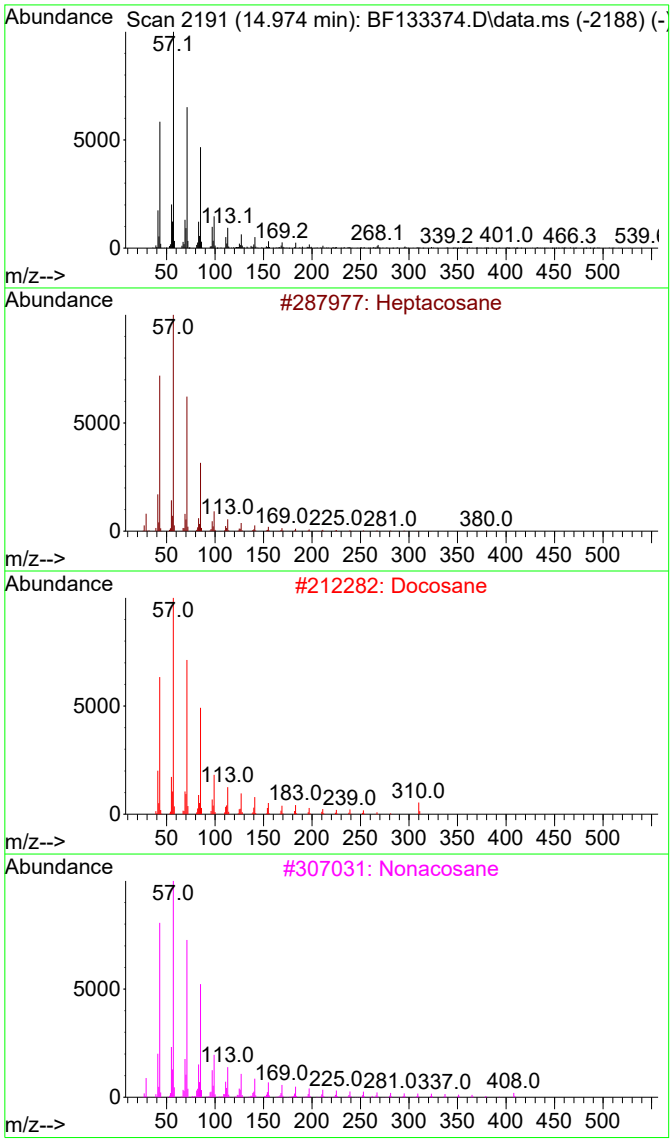
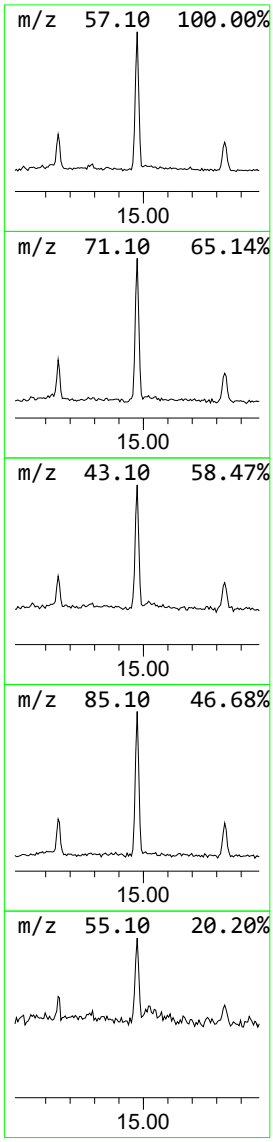
Peak Number 8 Heptacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.974	19.96 ng	584197	Perylene-d12	15.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	98
2	Docosane	310	C22H46	000629-97-0	97
3	Nonacosane	408	C29H60	000630-03-5	95
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
5	Heneicosane	296	C21H44	000629-94-7	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051223\
Data File : BF133374.D
Acq On : 12 May 2023 17:45
Operator : CG\JU
Sample : 02747-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-0-2-20230510

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

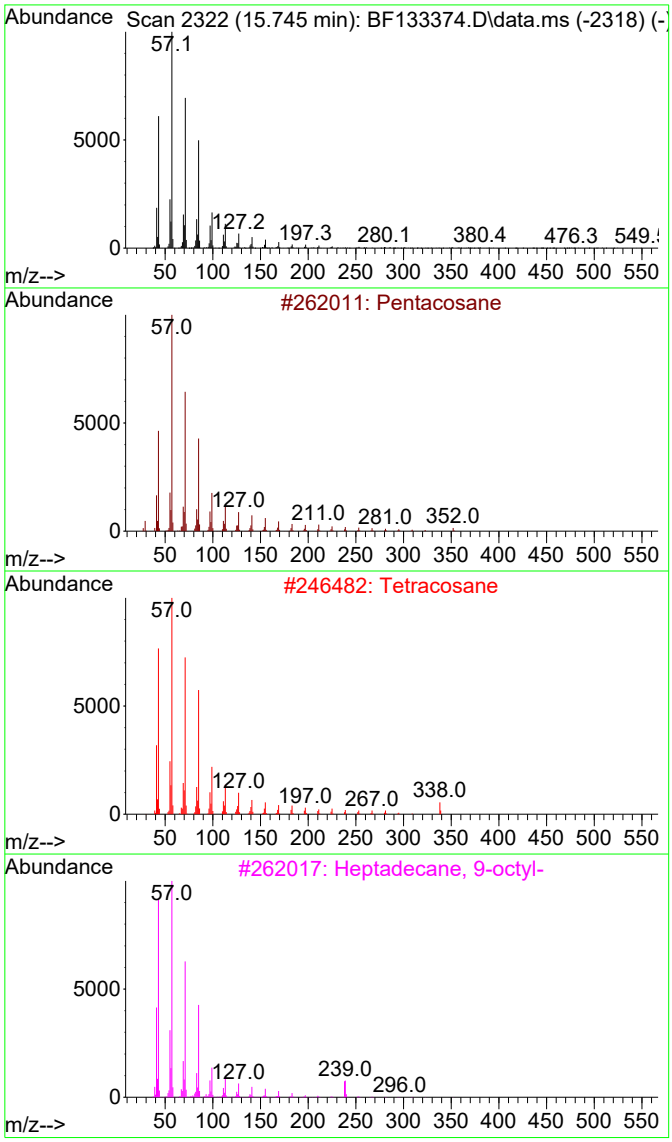
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

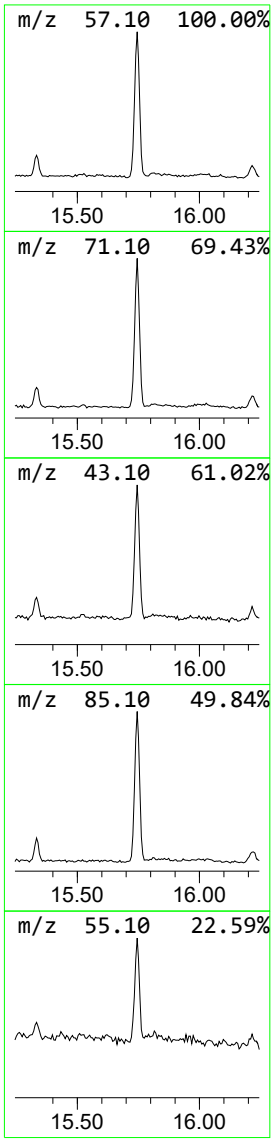
****

Peak Number 9 Pentacosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.745	43.38 ng	1269510	Perylene-d12	15.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	97
2	Tetracosane	338	C24H50	000646-31-1	96
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
4	Heptacosane	380	C27H56	000593-49-7	95
5	Tricosane	324	C23H48	000638-67-5	95





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051223\
Data File : BF133374.D
Acq On : 12 May 2023 17:45
Operator : CG\JU
Sample : 02747-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-0-2-20230510

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
2-Pentanone, 4-...	4.898	3.2	ng	172019	1	6.722	1089510	20.0
Caryophyllene	9.416	2.5	ng	202790	3	9.757	1642330	20.0
n-Hexadecanoic ...	11.774	11.0	ng	649446	4	11.239	1178810	20.0
Octadecanoic acid	12.563	4.2	ng	287716	5	13.874	1361490	20.0
1-Heptadecene	13.733	6.1	ng	416823	5	13.874	1361490	20.0
Docosane, 11-bu...	14.051	2.7	ng	181287	5	13.874	1361490	20.0
Docosane	14.357	2.1	ng	146254	5	13.874	1361490	20.0
Heptacosane	14.974	20.0	ng	584197	6	15.298	585328	20.0
Pentacosane	15.745	43.4	ng	1269510	6	15.298	585328	20.0