LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
Data File : BF121060.D
Acq On : 28 Jul 2020 10:18
Operator : JU/CG
Sample : L3435-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3

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-BF071620.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	498	502	509	rVB	46837	65206	1.21%	0.171%
2	5.434	563	569	572	rBV	3229996	3759391	69.53%	9.865%
3	6.445	735	741	744	rBV	3128732	3795024	70.19%	9.959%
4	6.645	772	775	785	rBV	37746	60736	1.12%	0.159%
5	6.810	800	803	807	rVB	1140196	879539	16.27%	2.308%
6	7.375	894	899	902	rBV	2506447	2603799	48.16%	6.833%
7	8.092	1017	1021	1025	rBV	1336778	1134218	20.98%	2.976%
8	9.175	1199	1205	1208	rBV	3937632	4426286	81.87%	11.615%
9	9.286	1222	1224	1232	rVB	46817	55855	1.03%	0.147%
10	9.563	1267	1271	1281	rBV	634376	548106	10.14%	1.438%
11	9.845	1315	1319	1334	rBV	1453993	1379952	25.52%	3.621%
12	10.639	1448	1454	1467	rBV	2604804	3161586	58.48%	8.296%
13	10.733	1468	1470	1476	rVV4	41110	76455	1.41%	0.201%
14	11.333	1567	1572	1577	rBV	1514863	1525577	28.22%	4.003%
15	11.722	1634	1638	1646	rVB	68368	84489	1.56%	0.222%
16	11.863	1657	1662	1670	rBV	476979	542551	10.03%	1.424%
17	12.057	1690	1695	1701	rVB4	66659	108422	2.01%	0.285%
18	12.310	1732	1738	1741	rBV	107042	106976	1.98%	0.281%
19	12.510	1769	1772	1777	rBV	80567	98514	1.82%	0.259%
20	12.645	1791	1795	1804	rBV	93112	118916	2.20%	0.312%
21	12.922	1836	1842	1845	rBV2	4294858	5406648	100.00%	14.188%
22	12.980	1845	1852	1865	rVB	250927	737586	13.64%	1.936%
23	13.145	1876	1880	1888	rVB2	48976	78929	1.46%	0.207%
24	13.492	1933	1939	1942	rBV2	50963	62466	1.16%	0.164%
25	13.816	1990	1994	2002	rBV	973423	1397311	25.84%	3.667%
26	13.892	2002	2007	2014	rVV	296116	564854	10.45%	1.482%
27	13.968	2015	2020	2032	rVB	1623732	1711997	31.66%	4.492%
28	14.133	2045	2048	2060	rVB2	80429	103669	1.92%	0.272%
29	14.345	2076	2084	2091	rBV10	34309	97460	1.80%	0.256%
30	14.439	2095	2100	2101	rBV2	98384	106427	1.97%	0.279%
31	14.545	2112	2118	2125	rBV	160132	297176	5.50%	0.780%
32	14.739	2147	2151	2155	rBV	117047	125258	2.32%	0.329%
33	14.816	2160	2164	2168	rVB	43209	59986	1.11%	0.157%
34	15.074	2203	2208	2212	rVB	134373	165316	3.06%	0.434%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
Data File : BF121060.D
Acq On : 28 Jul 2020 10:18
Operator : JU/CG
Sample : L3435-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3

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-BF071620.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.168	2218	2224	2236	rVB5	69625	224013	4.14%	0.588%
36	15.415	2260	2266	2270	rBV	1223478	1655128	30.61%	4.343%
37	15.868	2338	2343	2348	rBV	101295	185532	3.43%	0.487%
38	15.927	2348	2353	2362	rVV2	138539	351385	6.50%	0.922%
39	16.362	2421	2427	2431	rBV2	53211	100098	1.85%	0.263%
40	16.939	2519	2525	2532	rVB2	33868	74565	1.38%	0.196%
41	17.051	2537	2544	2545	rBV6	39578	70741	1.31%	0.186%

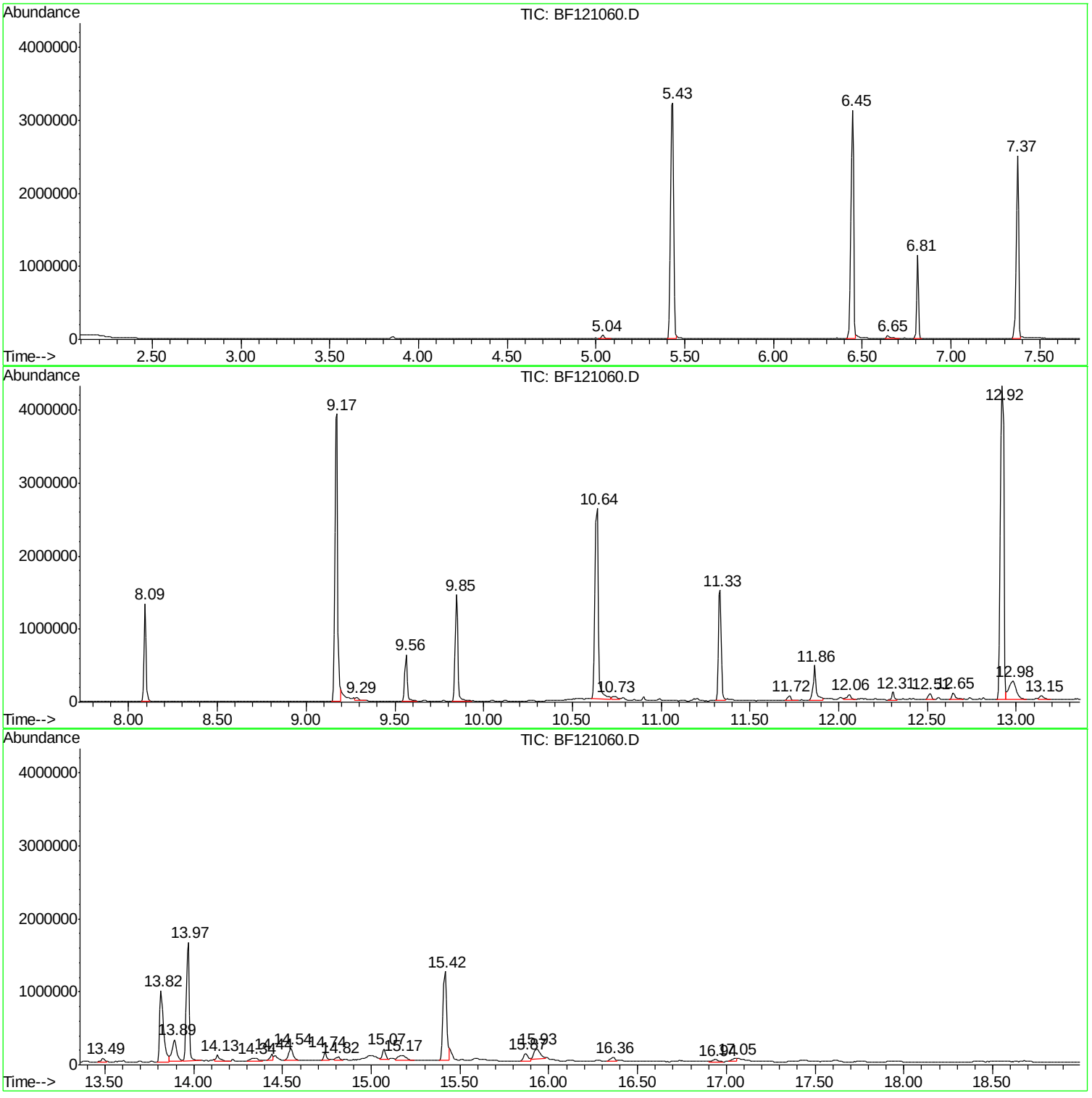
Sum of corrected areas: 38108143

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
Data File : BF121060.D
Acq On : 28 Jul 2020 10:18
Operator : JU/CG
Sample : L3435-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
Data File : BF121060.D
Acq On : 28 Jul 2020 10:18
Operator : JU/CG
Sample : L3435-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

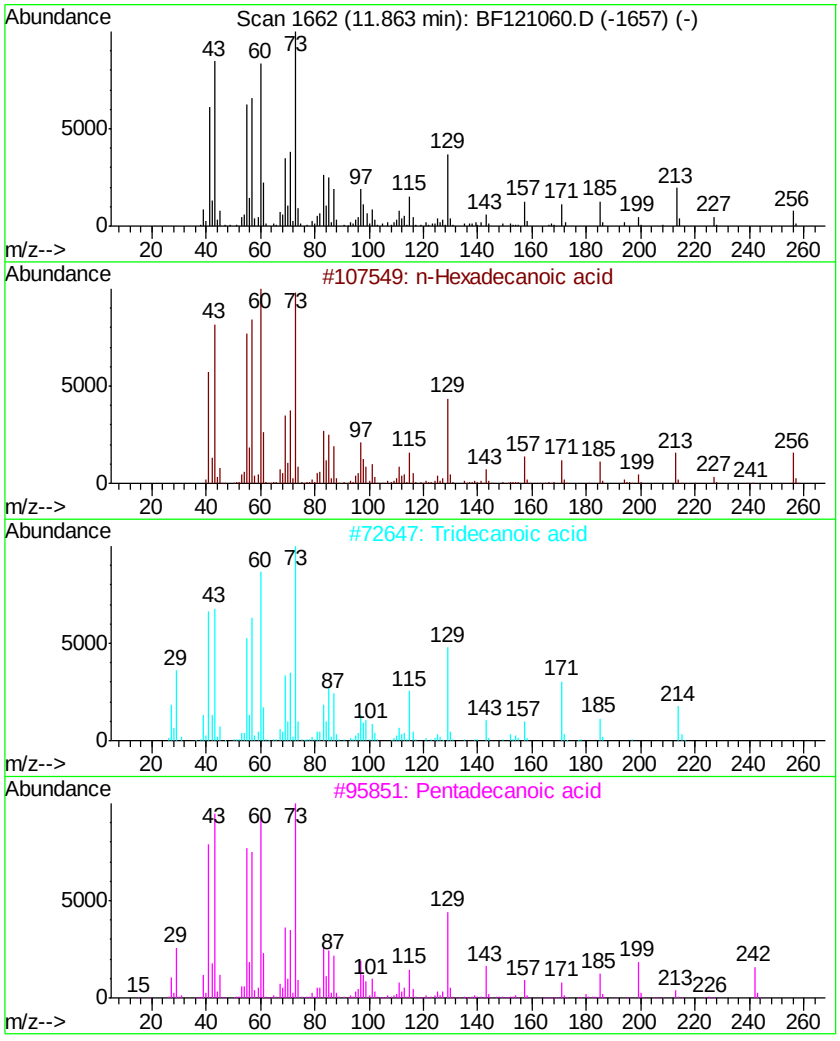
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

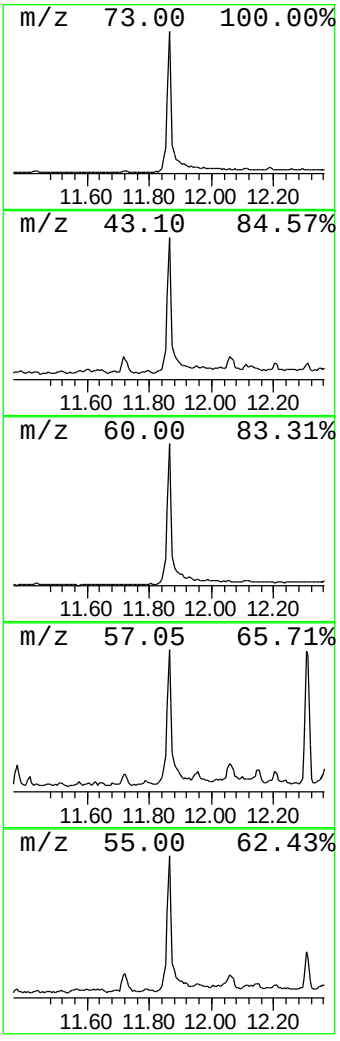
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	7.11 ng	542551	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
Data File : BF121060.D
Acq On : 28 Jul 2020 10:18
Operator : JU/CG
Sample : L3435-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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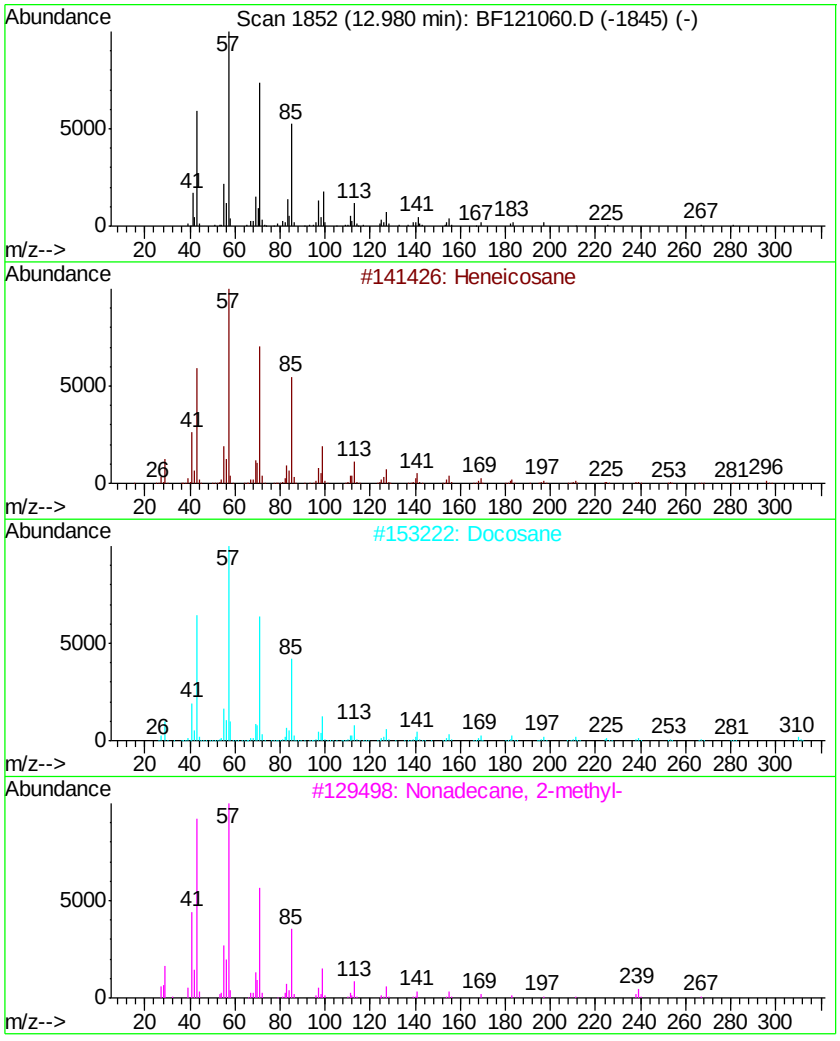
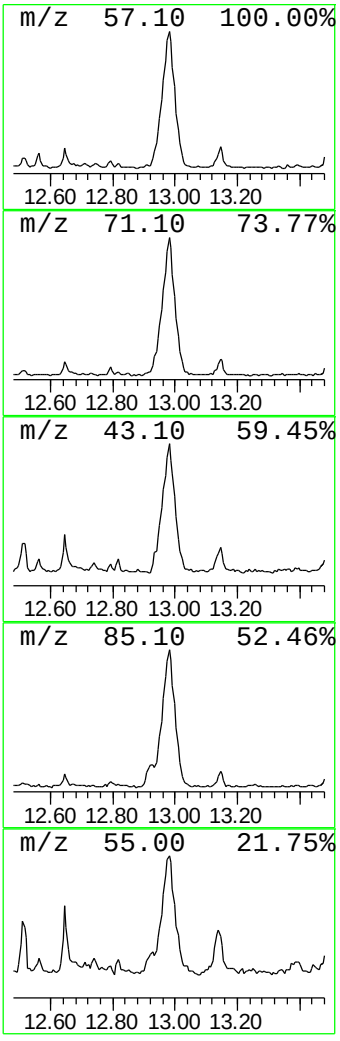
Peak Number 2 Heneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.98	8.62 ng	737586	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Docosane	310	C22H46	000629-97-0	90
3	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5	Pentacosane	352	C25H52	000629-99-2	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
Data File : BF121060.D
Acq On : 28 Jul 2020 10:18
Operator : JU/CG
Sample : L3435-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

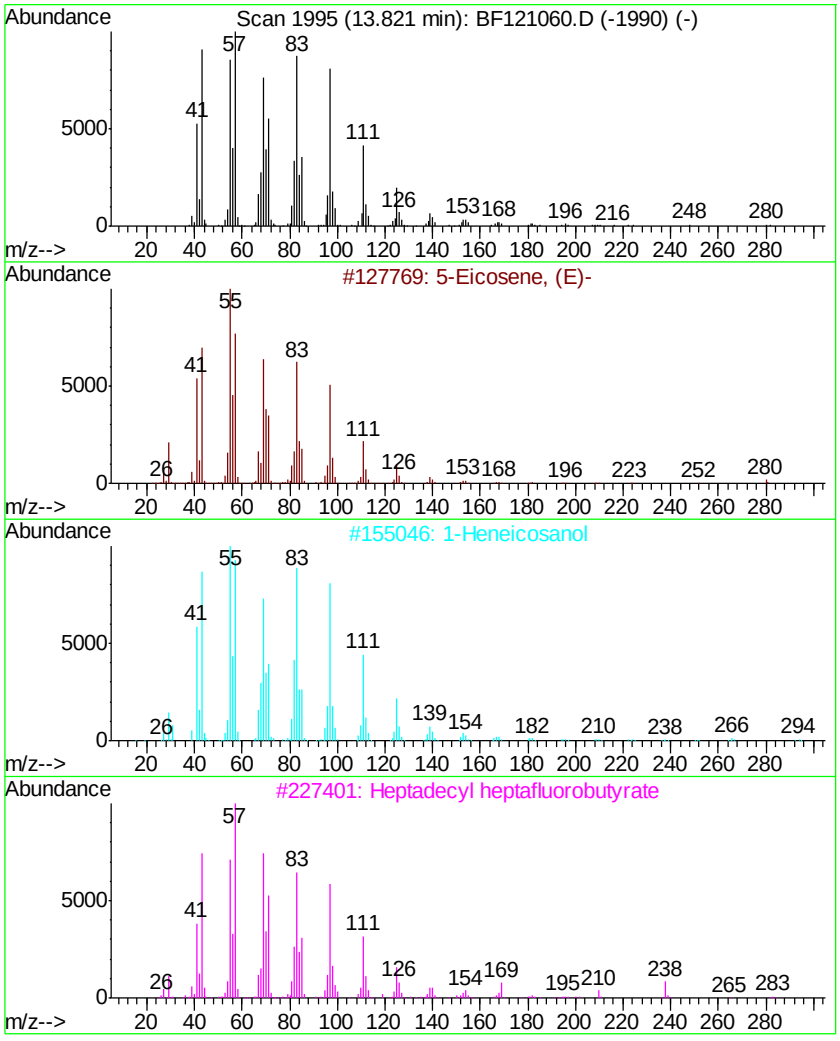
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

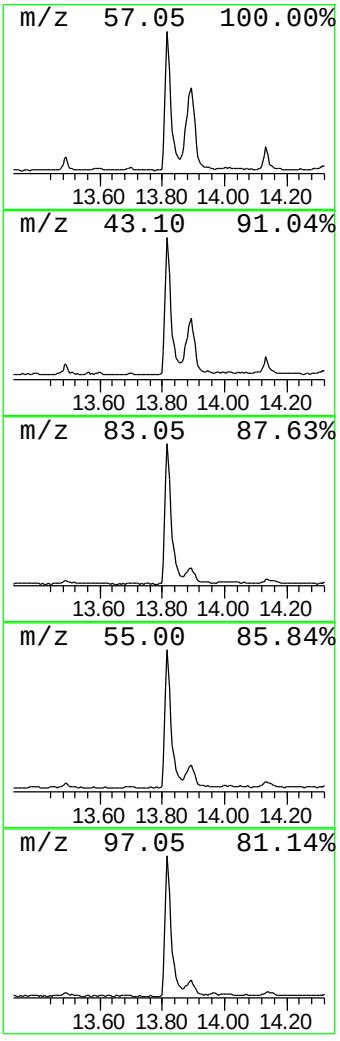
****

Peak Number 3 5-Eicosene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	16.32 ng	1397310	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
Data File : BF121060.D
Acq On : 28 Jul 2020 10:18
Operator : JU/CG
Sample : L3435-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

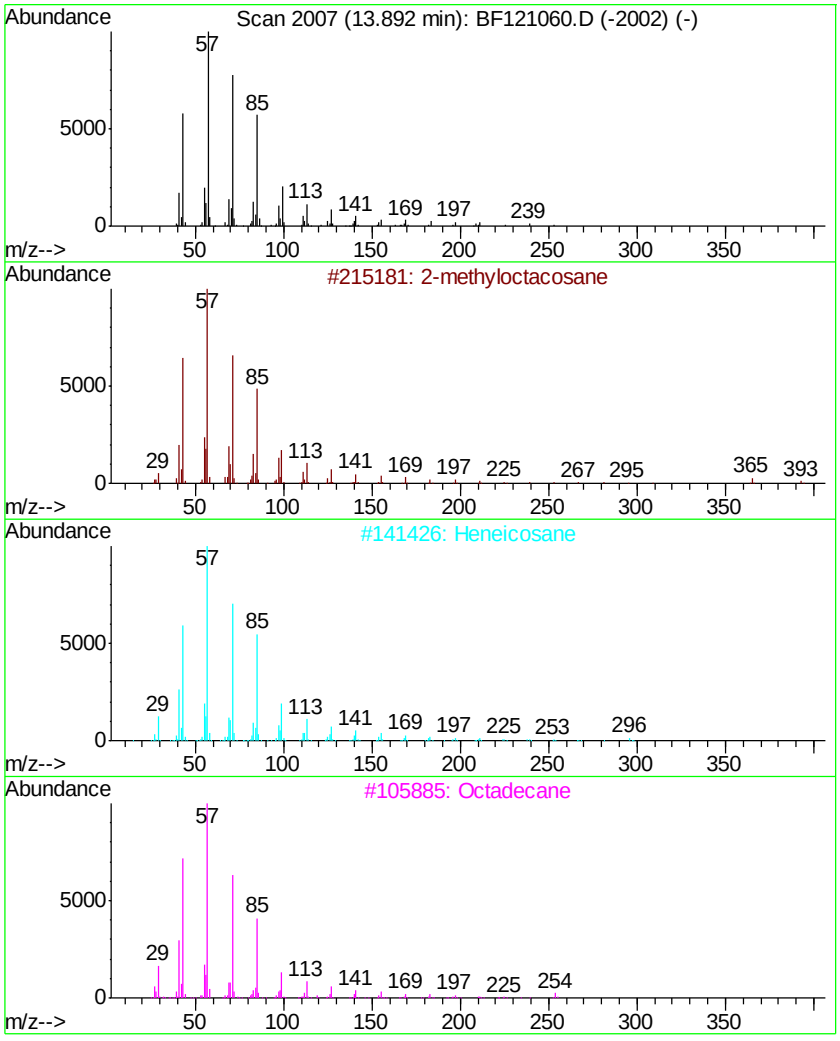
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

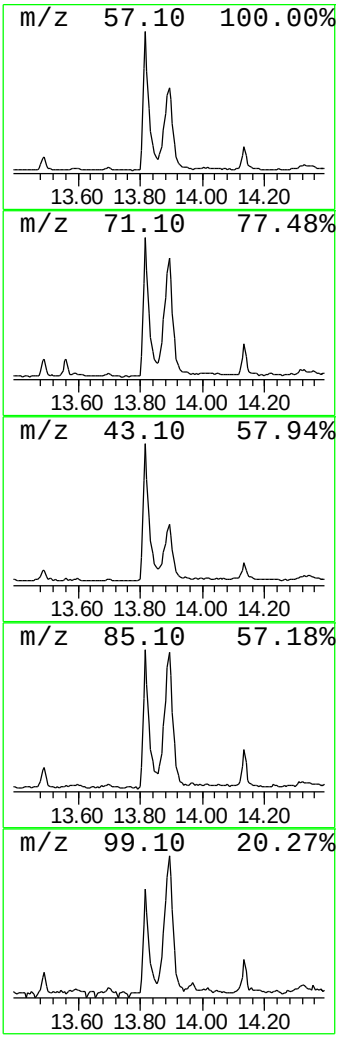
****

Peak Number 4 2-methyloctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	6.60 ng	564854	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octadecane	254	C18H38	000593-45-3	83
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	80
5	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	80





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
Data File : BF121060.D
Acq On : 28 Jul 2020 10:18
Operator : JU/CG
Sample : L3435-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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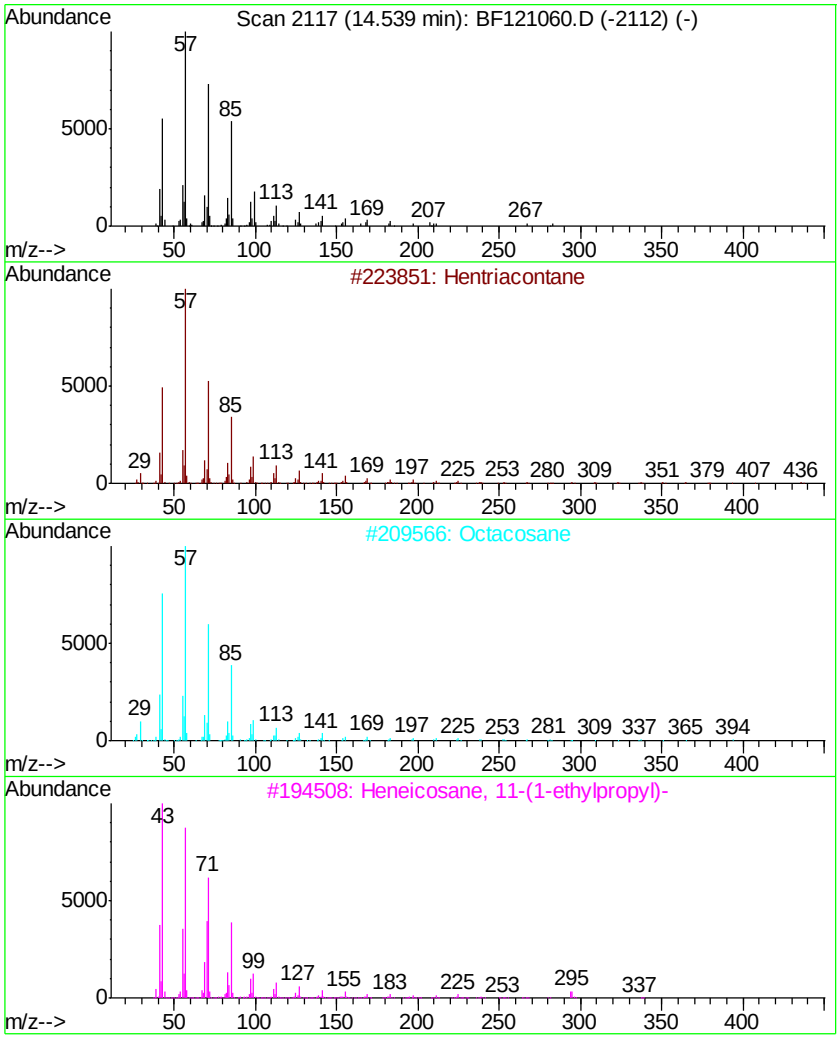
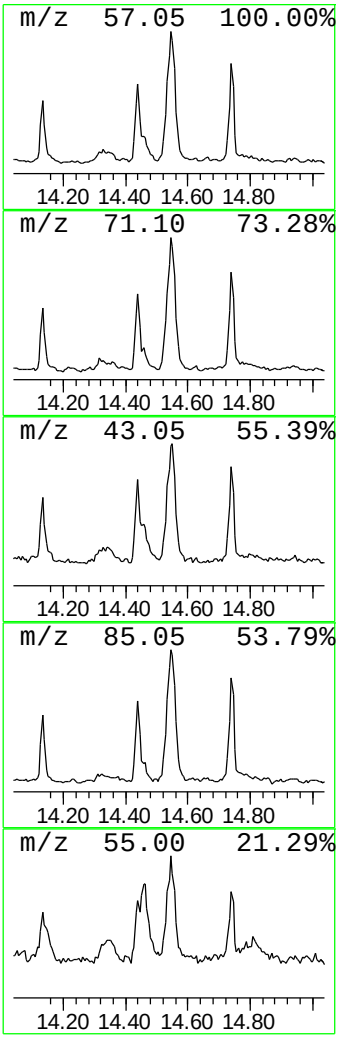
Peak Number 5 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	3.47 ng	297176	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Docosane	310	C22H46	000629-97-0	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
Data File : BF121060.D
Acq On : 28 Jul 2020 10:18
Operator : JU/CG
Sample : L3435-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

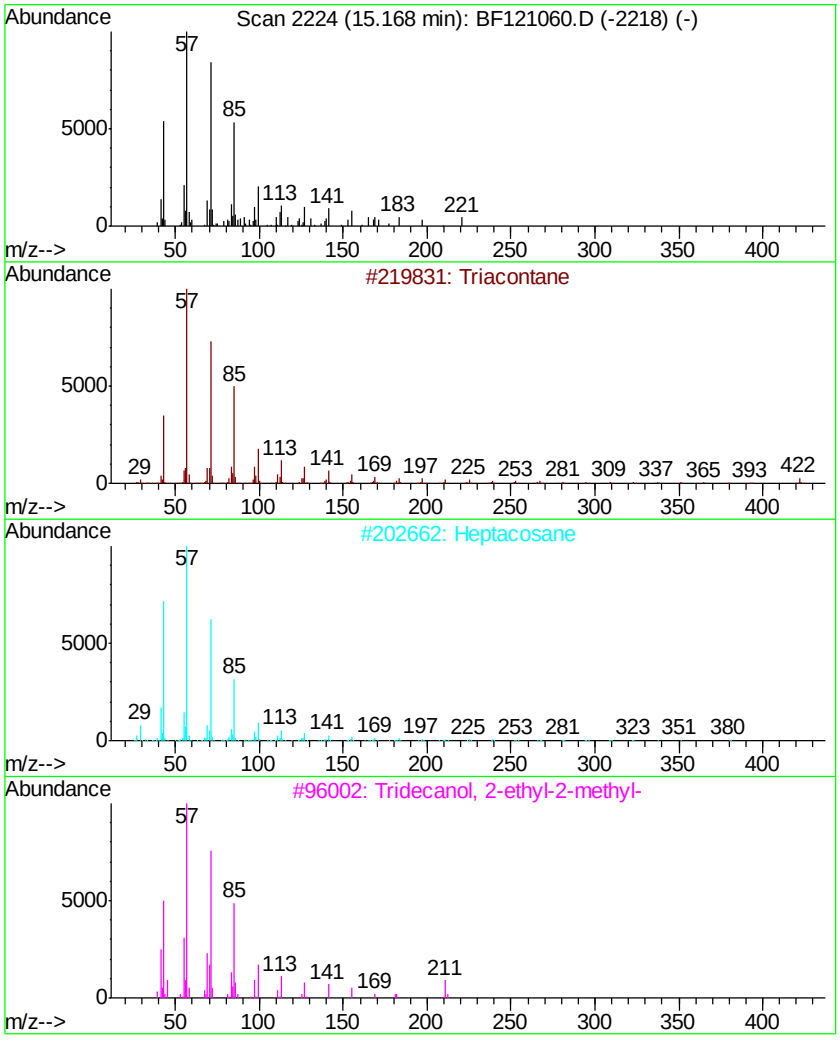
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

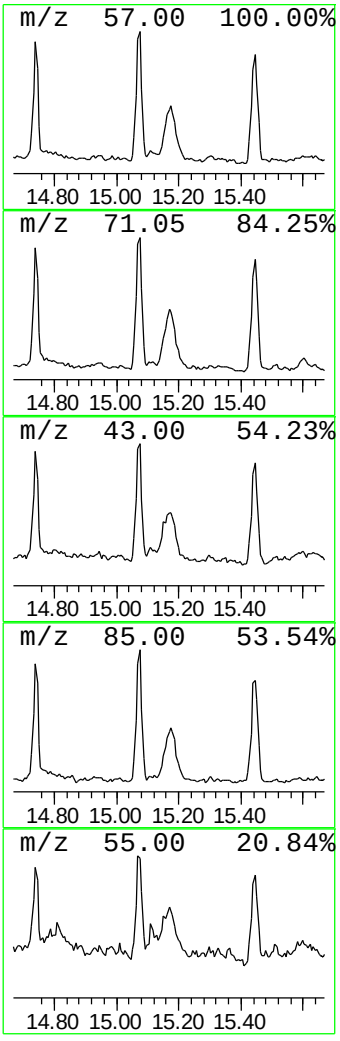
****

Peak Number 6 Triacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	2.71 ng	224013	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	90
2	Heptacosane	380	C27H56	000593-49-7	83
3	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	78
4	Hexadecane	226	C16H34	000544-76-3	64
5	Octadecane	254	C18H38	000593-45-3	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
Data File : BF121060.D
Acq On : 28 Jul 2020 10:18
Operator : JU/CG
Sample : L3435-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

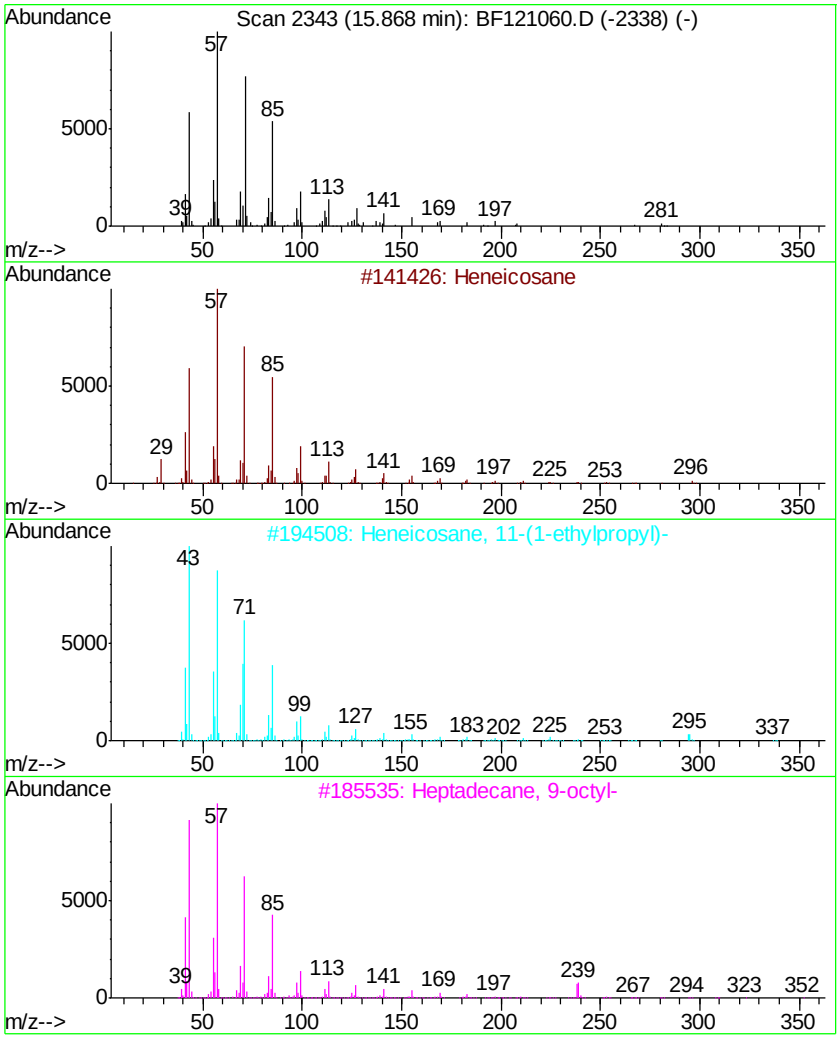
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

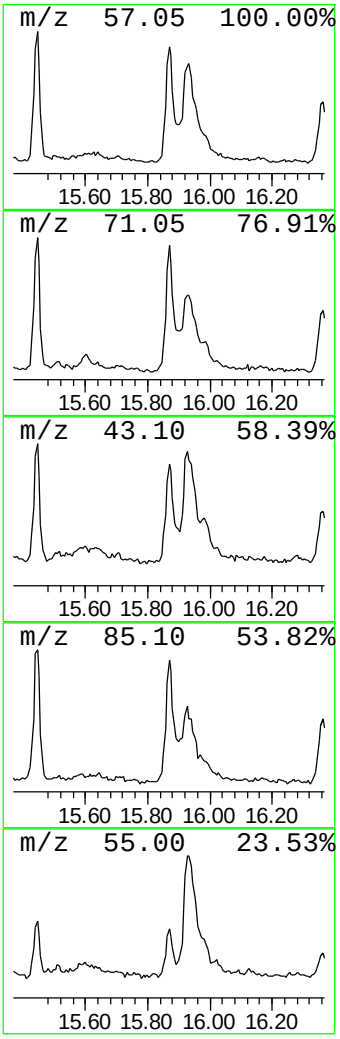
****

Peak Number 7 Heneicosane, 11-(1-ethylpro... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	2.24 ng	185532	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	91
5	Hexacosane	366	C26H54	000630-01-3	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
Data File : BF121060.D
Acq On : 28 Jul 2020 10:18
Operator : JU/CG
Sample : L3435-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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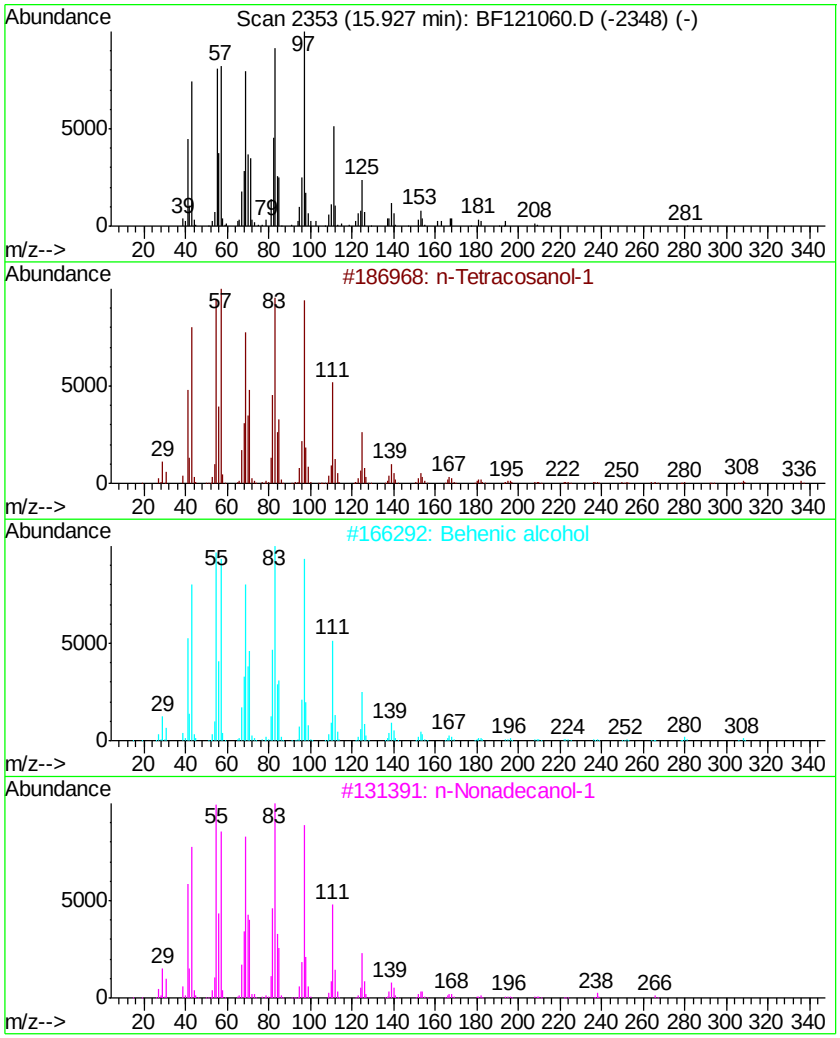
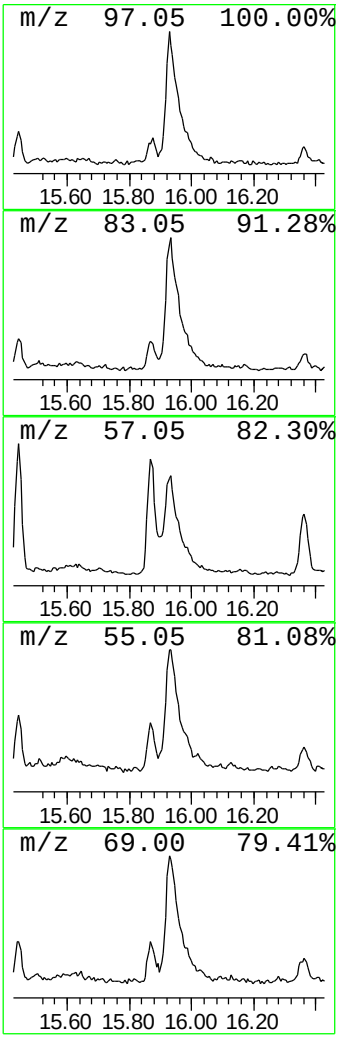
Peak Number 8 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	4.25 ng	351385	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072820\
Data File : BF121060.D
Acq On : 28 Jul 2020 10:18
Operator : JU/CG
Sample : L3435-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic acid	11.86	7.1	ng	542551	4	11.33	1525580	20.0
Heneicosane	12.98	8.6	ng	737586	5	13.97	1712000	20.0
5-Eicosene, (E)-	13.82	16.3	ng	1397310	5	13.97	1712000	20.0
2-methyloctacosane	13.89	6.6	ng	564854	5	13.97	1712000	20.0
Hentriacontane	14.54	3.5	ng	297176	5	13.97	1712000	20.0
Triacontane	15.17	2.7	ng	224013	6	15.42	1655130	20.0
Heneicosane, 11-(...	15.87	2.2	ng	185532	6	15.42	1655130	20.0
n-Tetracosanol-1	15.93	4.3	ng	351385	6	15.42	1655130	20.0