LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091620\
Data File : BF121593.D
Acq On : 16 Sep 2020 13:01
Operator : JU/CG
Sample : L3998-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-TEST1-ABCD-B

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-BF091020.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	5.045	498	503	510	rVB	87610	110124	2.11%	0.307%
2	5.445	567	571	575	rBV	3481413	3494940	66.98%	9.734%
3	6.457	739	743	757	rVB	3416767	3787515	72.59%	10.549%
4	6.651	773	776	783	rBV	93012	91444	1.75%	0.255%
5	6.822	801	805	808	rBV	1271350	992571	19.02%	2.764%
6	7.381	895	900	903	rBV	2476443	2522491	48.34%	7.025%
7	8.104	1018	1023	1026	rBV	1448847	1335401	25.59%	3.719%
8	9.181	1200	1206	1209	rBV	4385006	4377828	83.90%	12.193%
9	9.569	1268	1272	1276	rBV	453667	385123	7.38%	1.073%
10	9.857	1316	1321	1324	rBV	1805694	1587410	30.42%	4.421%
11	10.645	1449	1455	1458	rBV	3106982	3062734	58.70%	8.530%
12	11.339	1568	1573	1576	rBV	1910779	1720645	32.98%	4.792%
13	11.869	1656	1663	1675	rBV	655519	703639	13.49%	1.960%
14	12.551	1776	1779	1782	rBV	61992	55870	1.07%	0.156%
15	12.651	1793	1796	1809	rBV	171696	198820	3.81%	0.554%
16	12.774	1814	1817	1820	rVB	52292	52654	1.01%	0.147%
17	12.927	1837	1843	1846	rBV	5064014	5217718	100.00%	14.532%
18	13.157	1876	1882	1887	rBV4	43299	80651	1.55%	0.225%
19	13.498	1935	1940	1943	rBV2	65009	66457	1.27%	0.185%
20	13.821	1992	1995	2012	rBV	989183	1309080	25.09%	3.646%
21	13.974	2017	2021	2024	rBV	1767708	1706963	32.71%	4.754%
22	14.145	2046	2050	2060	rBV	96685	127753	2.45%	0.356%
23	14.451	2097	2102	2103	rBV3	114249	126727	2.43%	0.353%
24	14.751	2150	2153	2156	rVB	91587	84968	1.63%	0.237%
25	14.827	2162	2166	2170	rVB	243877	246662	4.73%	0.687%
26	15.086	2206	2210	2213	rBV	125504	141607	2.71%	0.394%
27	15.427	2263	2268	2272	rBV2	1104820	1397330	26.78%	3.892%
28	15.462	2272	2274	2279	rVB	111566	112634	2.16%	0.314%
29	15.892	2342	2347	2351	rBV	104915	150848	2.89%	0.420%
30	15.951	2352	2357	2379	rVB3	152960	411128	7.88%	1.145%
31	16.386	2427	2431	2435	rBV	53902	82272	1.58%	0.229%
32	16.962	2525	2529	2537	rVB2	47835	97879	1.88%	0.273%
33	17.080	2545	2549	2554	rBV6	26037	65252	1.25%	0.182%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091620\
Data File : BF121593.D
Acq On : 16 Sep 2020 13:01
Operator : JU/CG
Sample : L3998-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-TEST1-ABCD-B

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-BF091020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

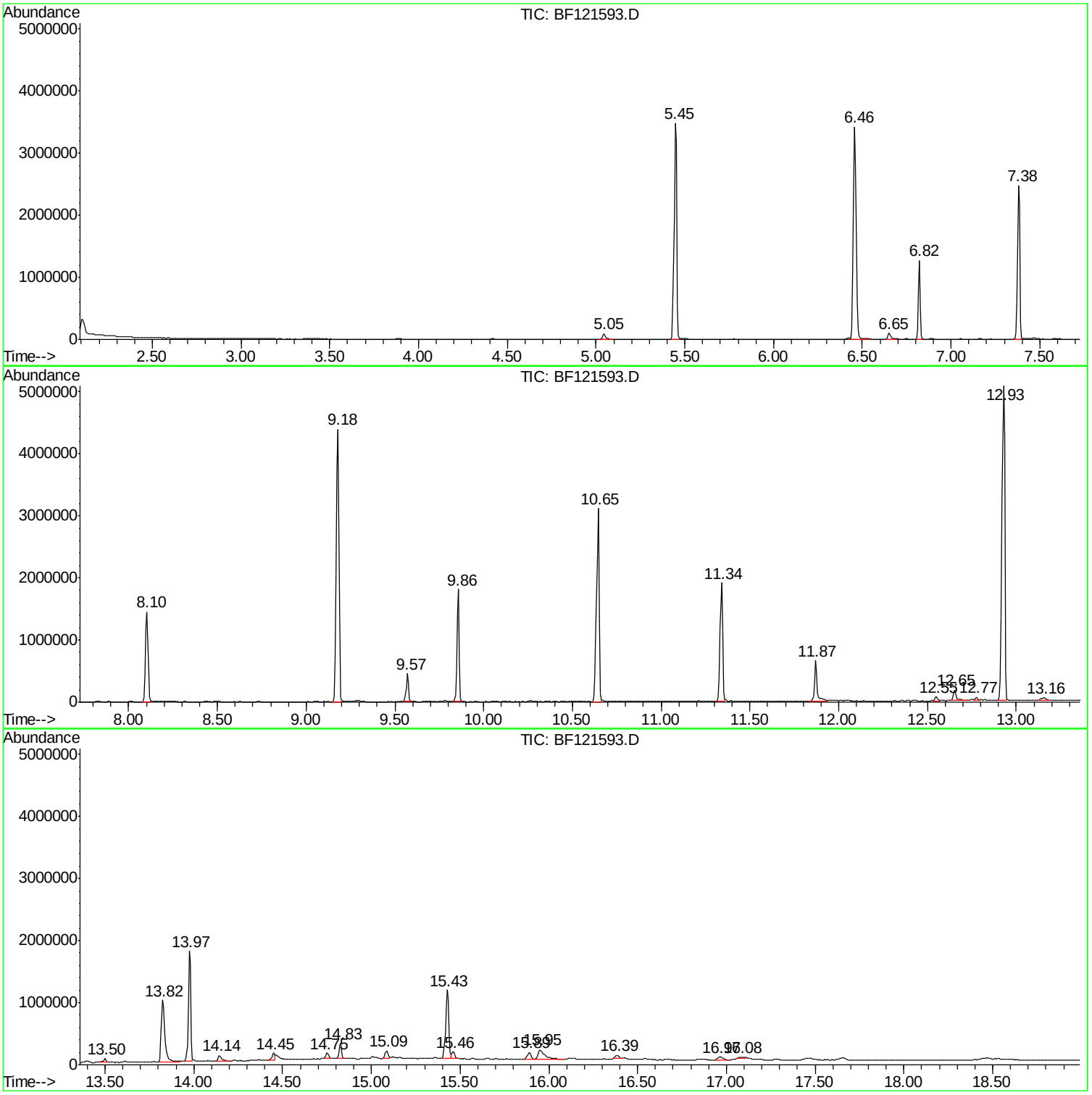
Sum of corrected areas: 35905138

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091620\
Data File : BF121593.D
Acq On : 16 Sep 2020 13:01
Operator : JU/CG
Sample : L3998-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-TEST1-ABCD-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091620\
Data File : BF121593.D
Acq On : 16 Sep 2020 13:01
Operator : JU/CG
Sample : L3998-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-TEST1-ABCD-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

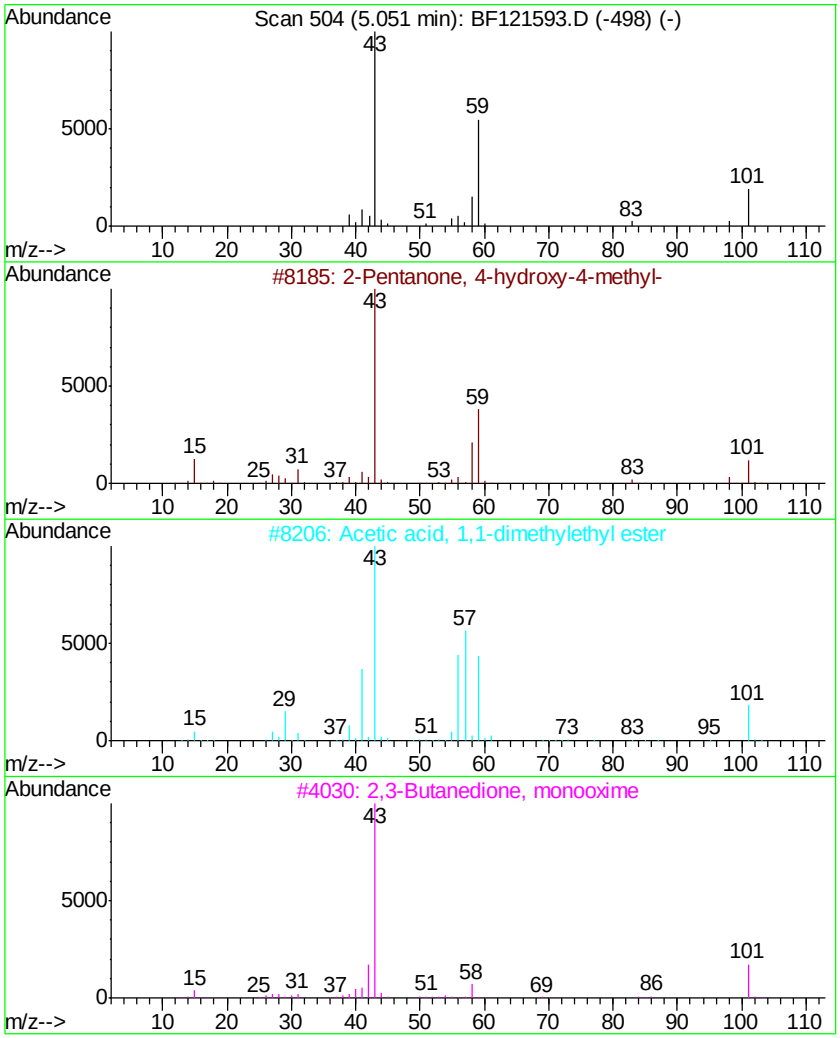
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

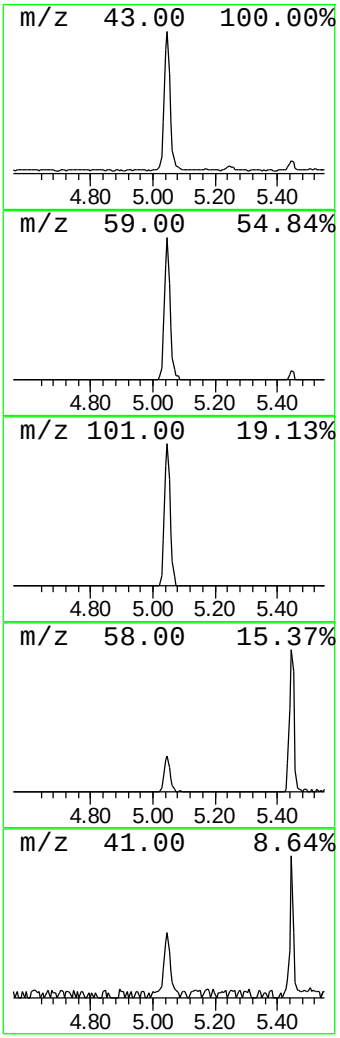
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	2.22 ng	110124	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091620\
Data File : BF121593.D
Acq On : 16 Sep 2020 13:01
Operator : JU/CG
Sample : L3998-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-TEST1-ABCD-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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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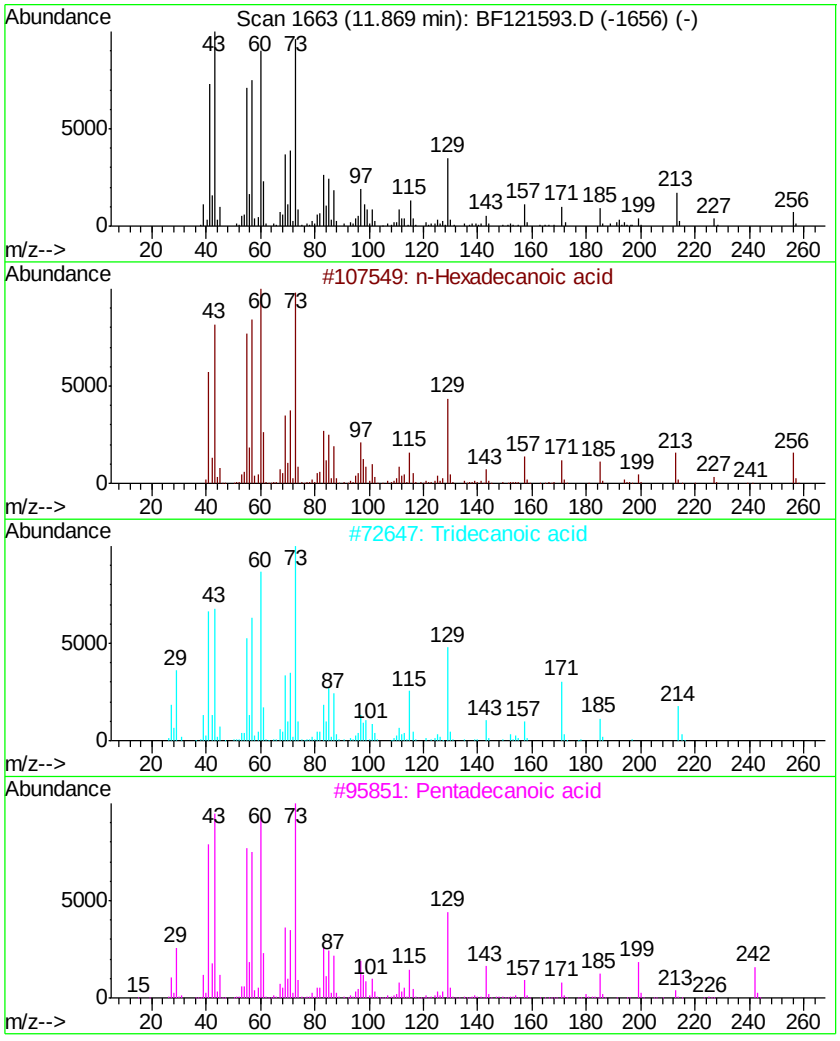
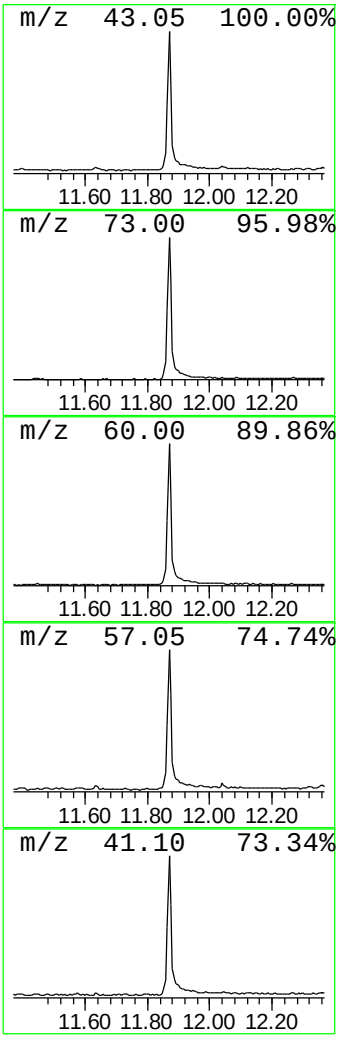
Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	8.18 ng	703639	Phenanthrene-d10	11.34

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	20





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091620\
Data File : BF121593.D
Acq On : 16 Sep 2020 13:01
Operator : JU/CG
Sample : L3998-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-TEST1-ABCD-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

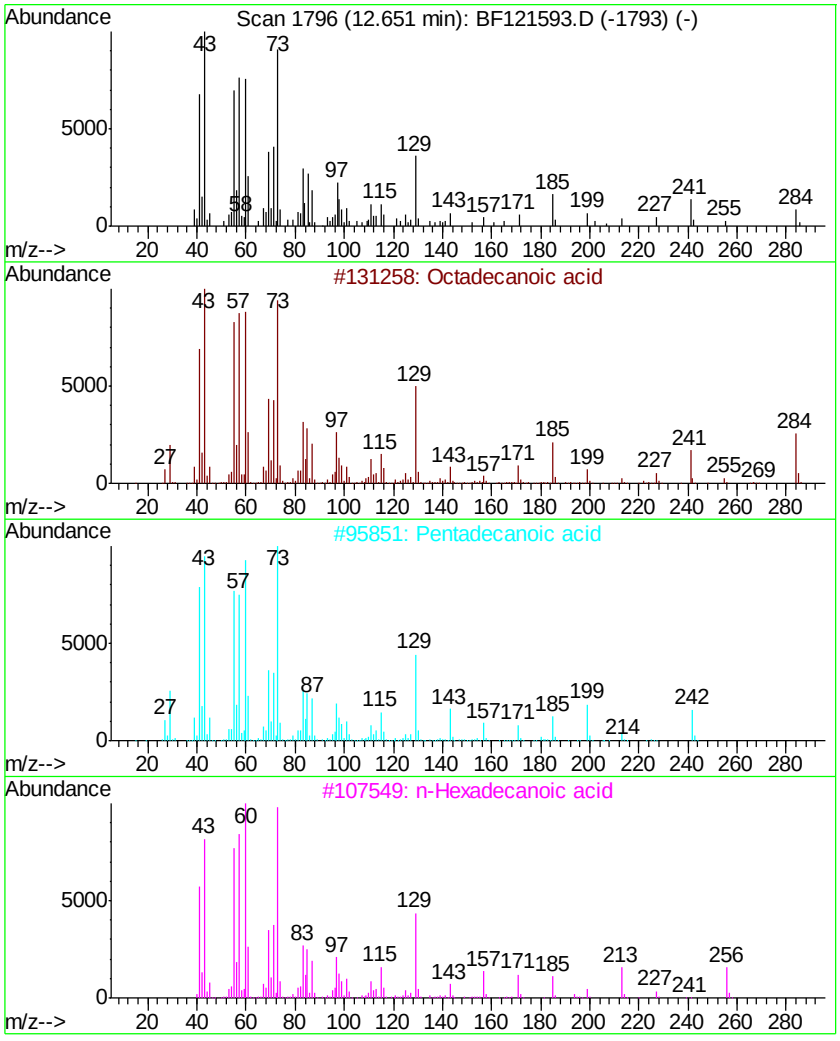
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

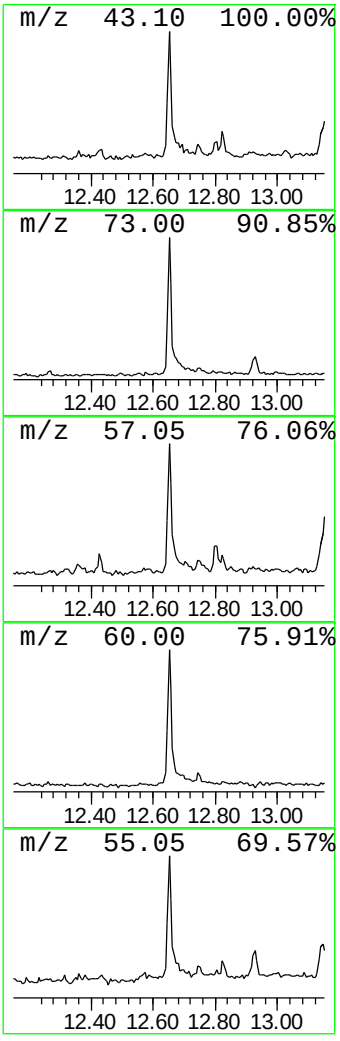
****

Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.31 ng	198820	Phenanthrene-d10	11.34

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	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091620\
Data File : BF121593.D
Acq On : 16 Sep 2020 13:01
Operator : JU/CG
Sample : L3998-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-TEST1-ABCD-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

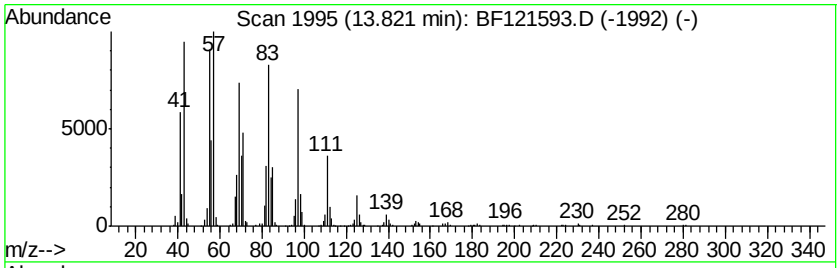
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

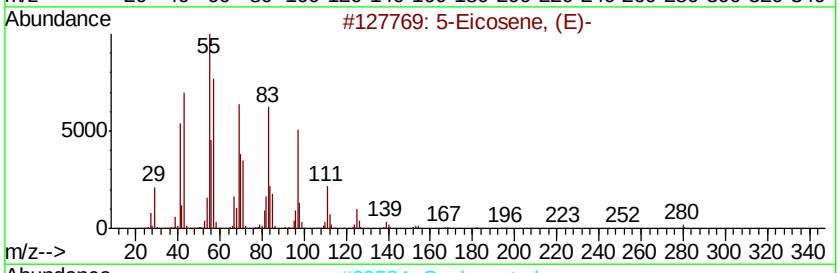
****

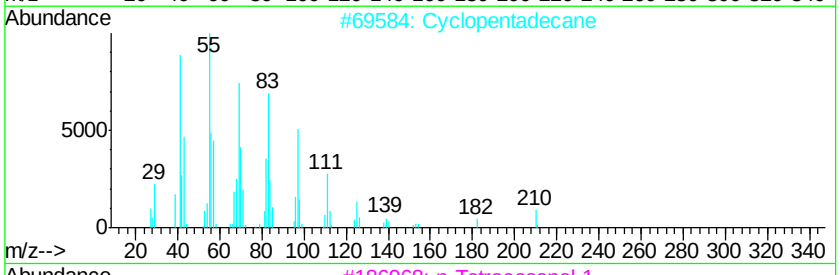
Peak Number 4 5-Eicosene, (E)- Concentration Rank 1

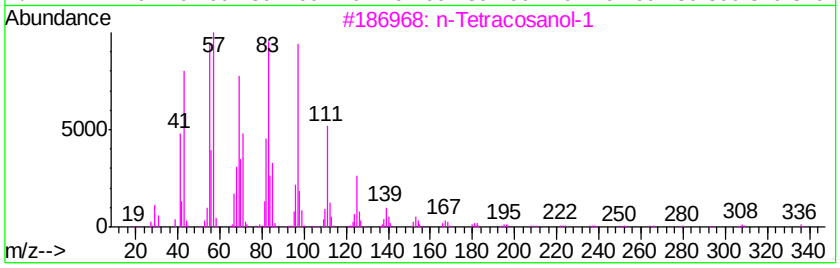
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	15.34 ng	1309080	Chrysene-d12	13.97

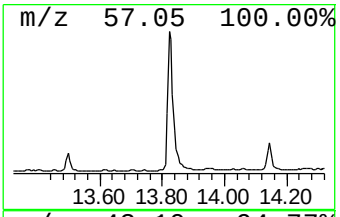
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	Cyclopentadecane	210	C15H30	000295-48-7	96
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93

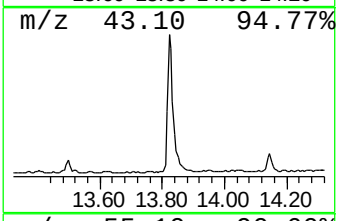


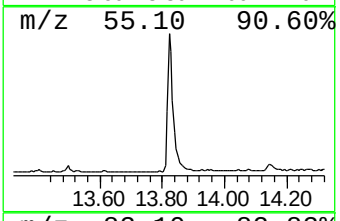


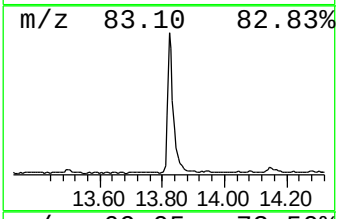


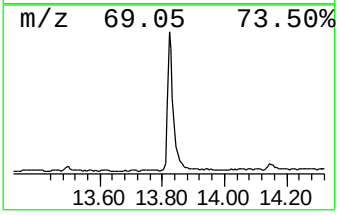












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091620\
Data File : BF121593.D
Acq On : 16 Sep 2020 13:01
Operator : JU/CG
Sample : L3998-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-TEST1-ABCD-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

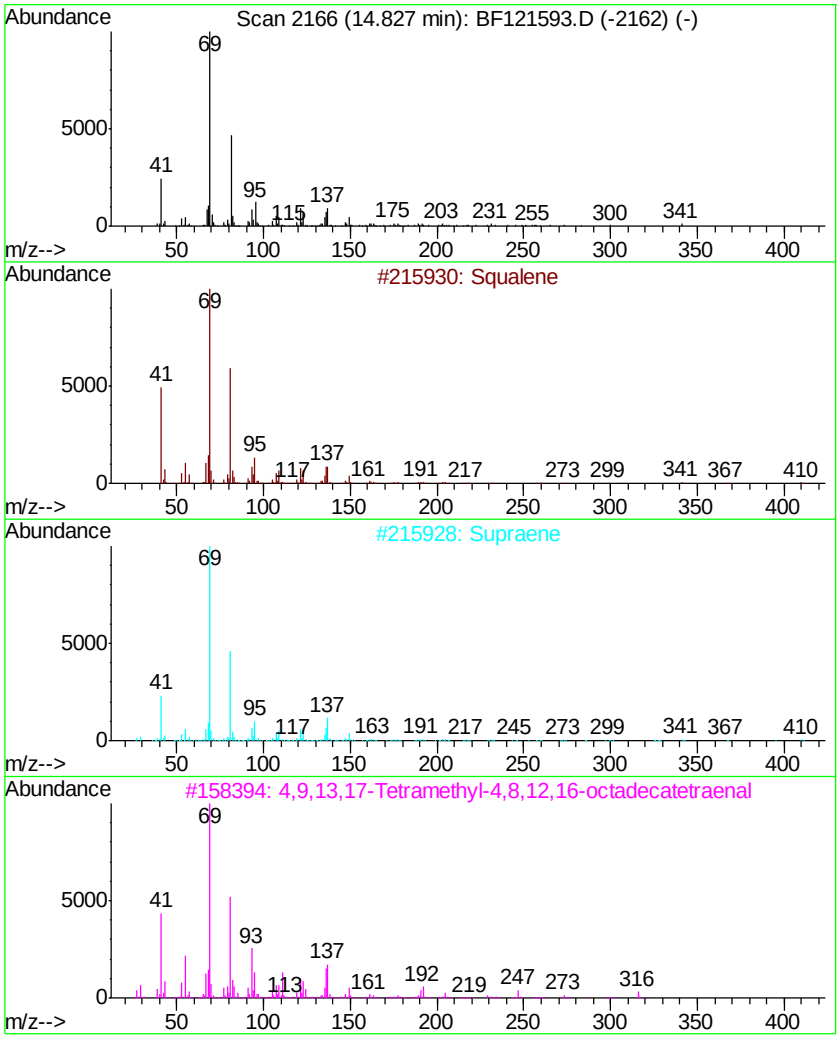
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

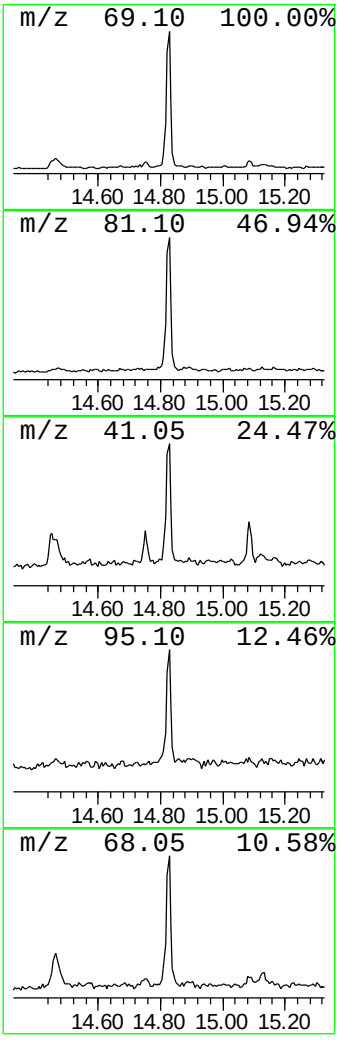
****

Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	3.53 ng	246662	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	87
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4	2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091620\
Data File : BF121593.D
Acq On : 16 Sep 2020 13:01
Operator : JU/CG
Sample : L3998-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-TEST1-ABCD-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

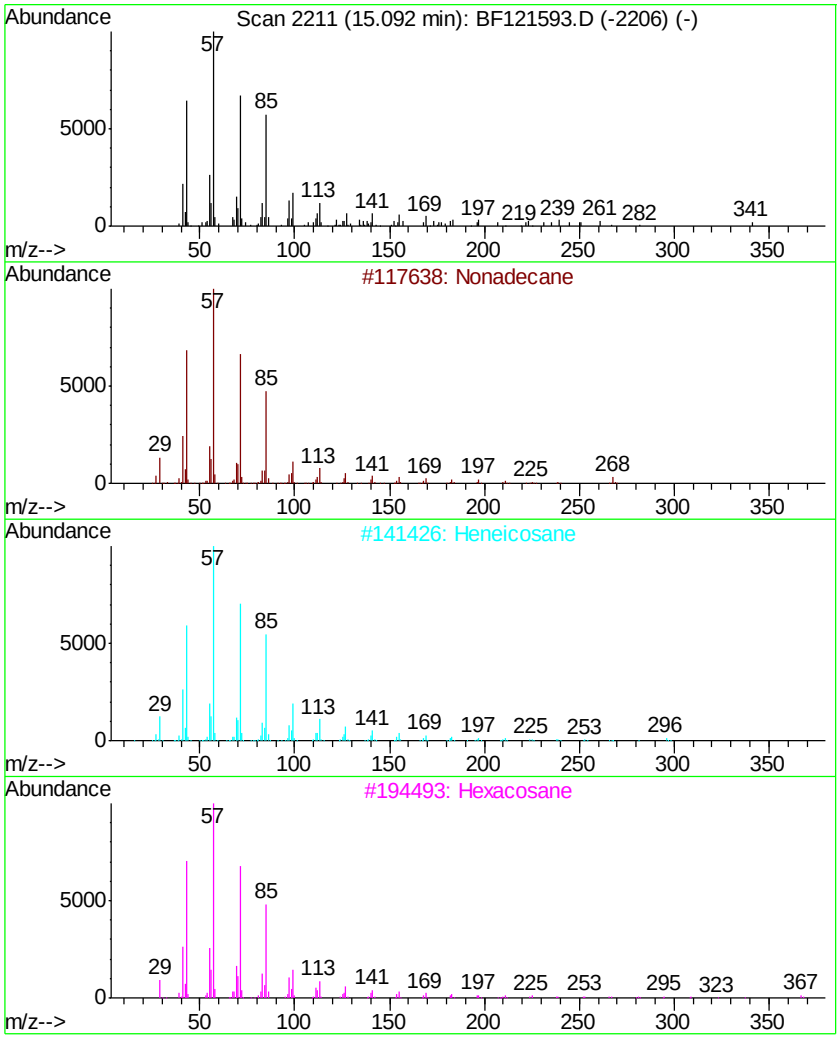
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

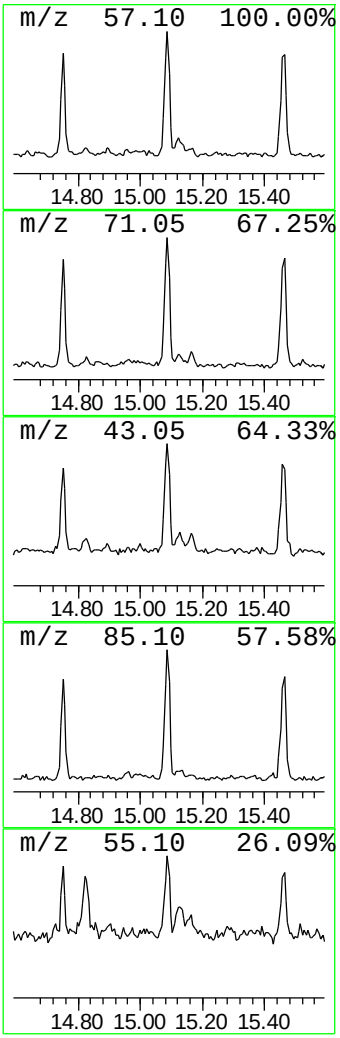
****

Peak Number 6 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	2.03 ng	141607	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Heneicosane	296	C21H44	000629-94-7	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Eicosane	282	C20H42	000112-95-8	87
5	Octacosane	394	C28H58	000630-02-4	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091620\
Data File : BF121593.D
Acq On : 16 Sep 2020 13:01
Operator : JU/CG
Sample : L3998-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-TEST1-ABCD-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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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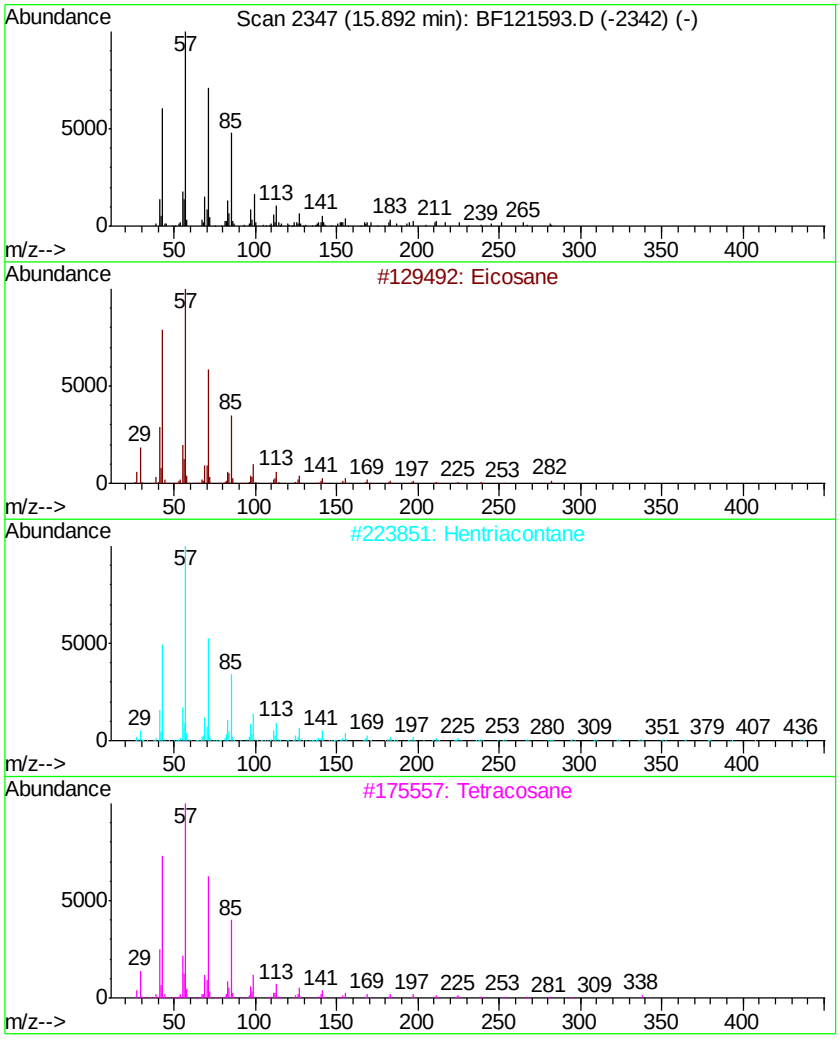
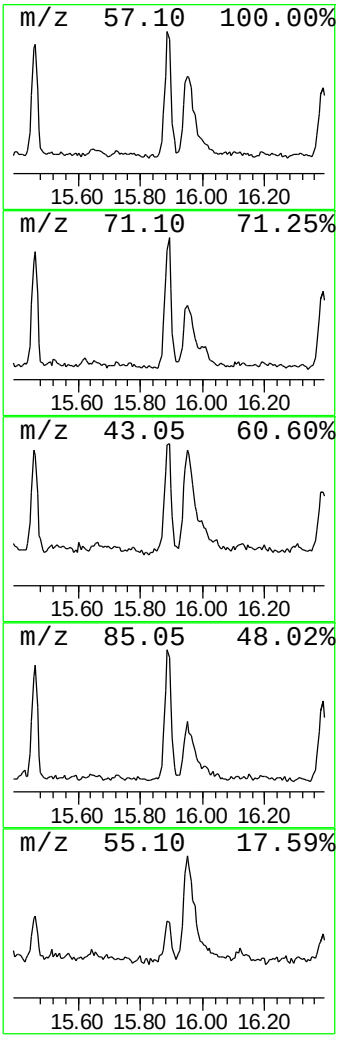
Peak Number 7 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	2.16 ng	150848	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Hentriacontane	437	C31H64	000630-04-6	90
3	Tetracosane	338	C24H50	000646-31-1	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Heneicosane	296	C21H44	000629-94-7	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091620\
Data File : BF121593.D
Acq On : 16 Sep 2020 13:01
Operator : JU/CG
Sample : L3998-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-TEST1-ABCD-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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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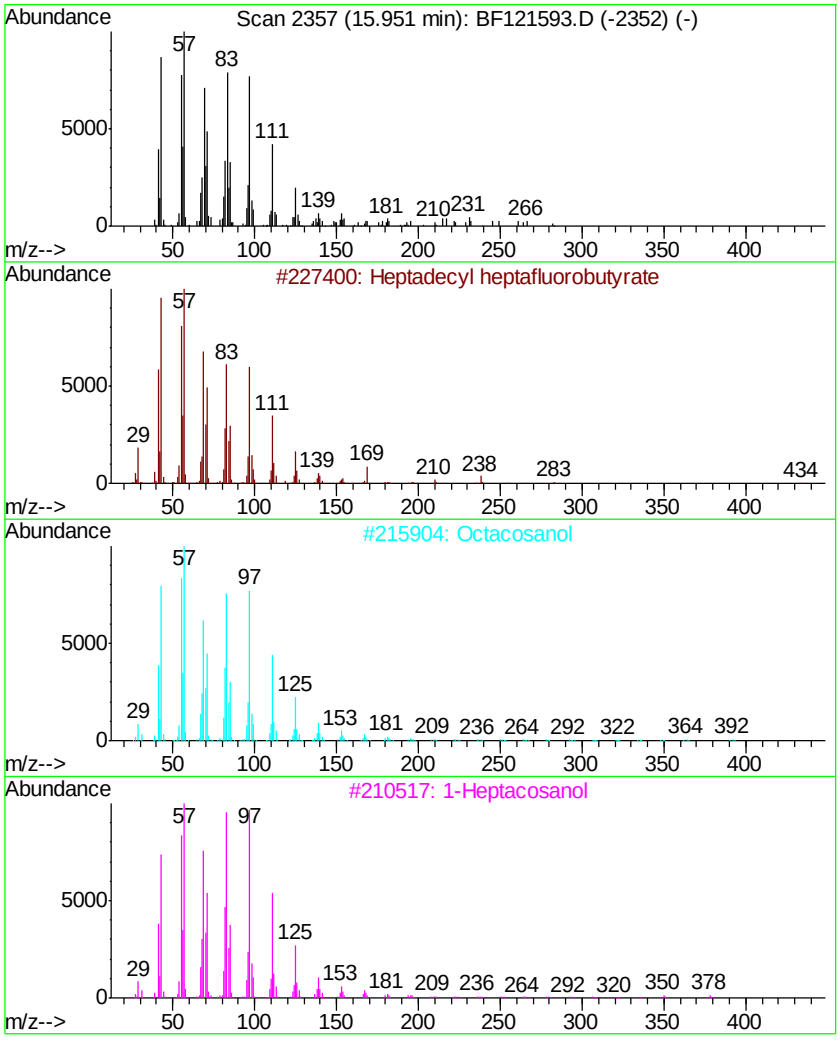
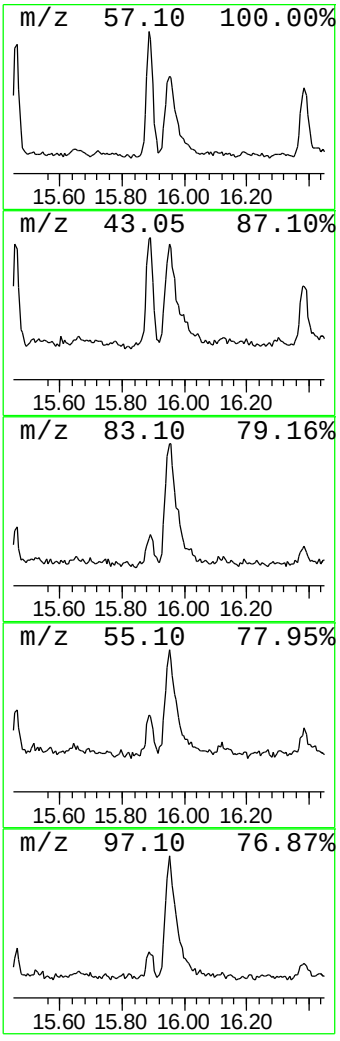
Peak Number 8 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	5.88 ng	411128	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Octacosanol	410	C28H58O	000557-61-9	94
3	1-Heptacosanol	396	C27H56O	002004-39-9	91
4	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
5	1-Docosene	308	C22H44	001599-67-3	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091620\
Data File : BF121593.D
Acq On : 16 Sep 2020 13:01
Operator : JU/CG
Sample : L3998-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-EF-01-TEST1-ABCD-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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
2-Pentanone, 4-hy...	5.05	2.2	ng	110124	1	6.82	992571	20.0
n-Hexadecanoic acid	11.87	8.2	ng	703639	4	11.34	1720650	20.0
Octadecanoic acid	12.65	2.3	ng	198820	4	11.34	1720650	20.0
5-Eicosene, (E)-	13.82	15.3	ng	1309080	5	13.97	1706960	20.0
Squalene	14.83	3.5	ng	246662	6	15.43	1397330	20.0
Nonadecane	15.09	2.0	ng	141607	6	15.43	1397330	20.0
Eicosane	15.89	2.2	ng	150848	6	15.43	1397330	20.0
Heptadecyl heptaf...	15.95	5.9	ng	411128	6	15.43	1397330	20.0