LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112985.D
Acq On : 12 Mar 2019 5:44
Operator : JU/SJ
Sample : K1817-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-027-B112-030719

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-BF022719.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	5.334	548	552	565	rBV	2308465	2335794	73.53%	8.183%
2	6.363	723	727	746	rBV	2471742	2679144	84.34%	9.386%
3	6.498	746	750	753	rBV	2999473	2557431	80.51%	8.959%
4	6.728	786	789	793	rBV	975522	788662	24.83%	2.763%
5	6.886	812	816	819	rBV	2342826	1929798	60.75%	6.761%
6	7.286	880	884	898	rBV	1618657	1589815	50.05%	5.570%
7	8.010	1003	1007	1014	rBV	880404	953170	30.01%	3.339%
8	9.086	1186	1190	1202	rBV	3112521	3044731	95.85%	10.666%
9	9.480	1253	1257	1268	rVB	244914	236312	7.44%	0.828%
10	9.763	1301	1305	1324	rBV	1293303	1236176	38.91%	4.331%
11	10.545	1434	1438	1453	rBV	2241873	2254469	70.97%	7.898%
12	11.239	1552	1556	1564	rBV	1404664	1390337	43.77%	4.871%
13	11.774	1644	1647	1658	rBV	249258	311918	9.82%	1.093%
14	12.445	1758	1761	1764	rBV	57928	52204	1.64%	0.183%
15	12.557	1778	1780	1793	rBV3	46763	81167	2.56%	0.284%
16	12.651	1793	1796	1797	rVV2	33472	32127	1.01%	0.113%
17	12.668	1797	1799	1803	rVB	46235	45589	1.44%	0.160%
18	12.815	1820	1824	1828	rBV	3176951	3176683	100.00%	11.129%
19	13.063	1860	1866	1870	rBV2	44380	55319	1.74%	0.194%
20	13.304	1904	1907	1912	rVB	68191	60750	1.91%	0.213%
21	13.404	1918	1924	1926	rBV2	54169	53915	1.70%	0.189%
22	13.727	1975	1979	1992	rBV	307825	493545	15.54%	1.729%
23	13.862	1998	2002	2018	rBV	1201770	1288843	40.57%	4.515%
24	14.045	2030	2033	2040	rBV	88217	89043	2.80%	0.312%
25	14.345	2081	2084	2087	rBV	110084	117292	3.69%	0.411%
26	14.639	2131	2134	2138	rBV	117244	119997	3.78%	0.420%
27	14.874	2171	2174	2182	rBV	23048	48212	1.52%	0.169%
28	14.957	2184	2188	2192	rBV	123934	142834	4.50%	0.500%
29	14.998	2192	2195	2199	rBV5	23933	40558	1.28%	0.142%
30	15.268	2236	2241	2246	rBV	687081	940046	29.59%	3.293%
31	15.309	2246	2248	2256	rVB	118220	157122	4.95%	0.550%
32	15.715	2313	2317	2324	rBV	87015	138488	4.36%	0.485%
33	16.186	2392	2397	2409	rVB3	48761	103392	3.25%	0.362%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112985.D
Acq On : 12 Mar 2019 5:44
Operator : JU/SJ
Sample : K1817-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PST-027-B112-030719

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-BF022719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

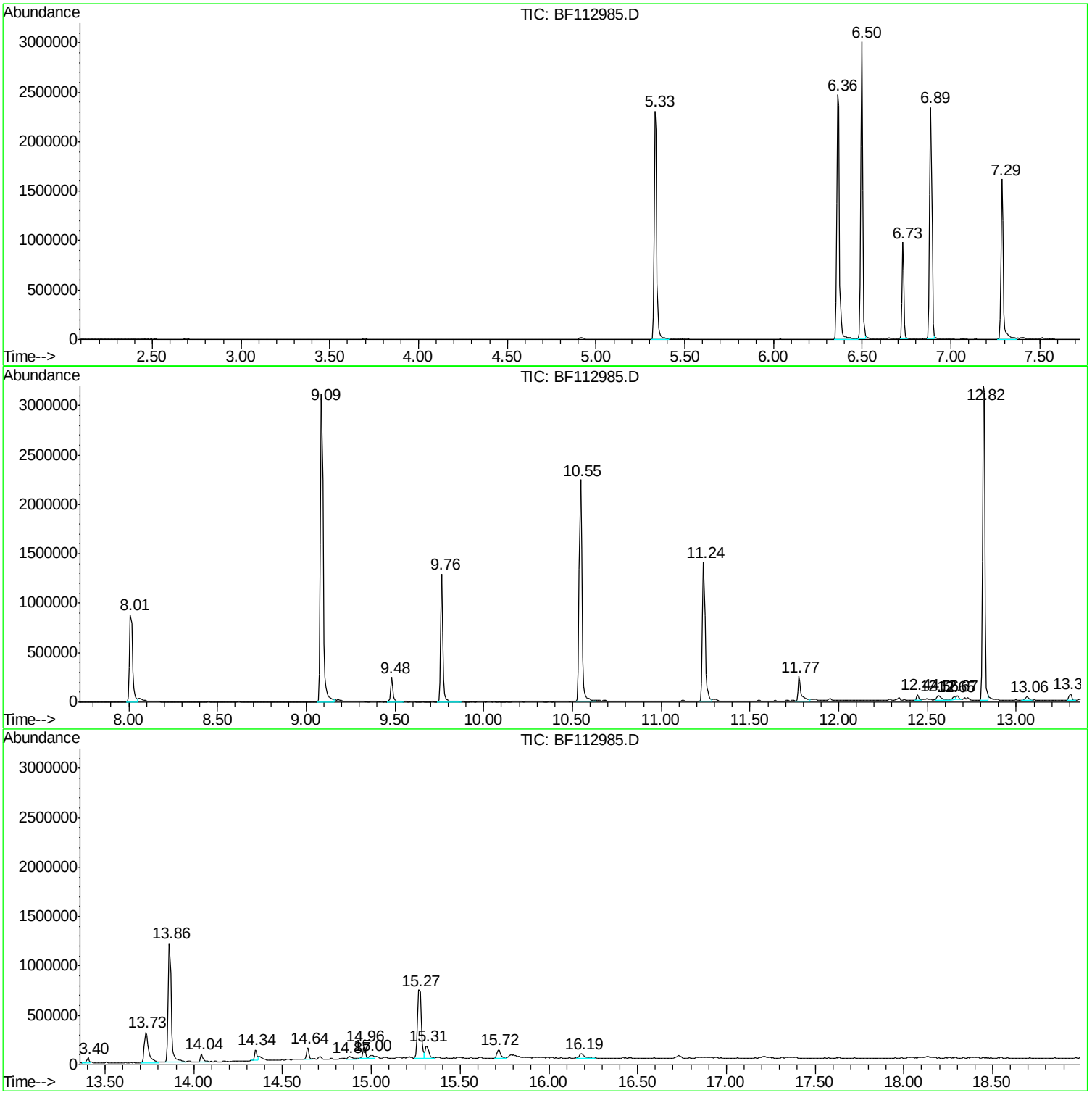
Sum of corrected areas: 28544883

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112985.D
Acq On : 12 Mar 2019 5:44
Operator : JU/SJ
Sample : K1817-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PST-027-B112-030719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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\BF031119\
Data File : BF112985.D
Acq On : 12 Mar 2019 5:44
Operator : JU/SJ
Sample : K1817-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-027-B112-030719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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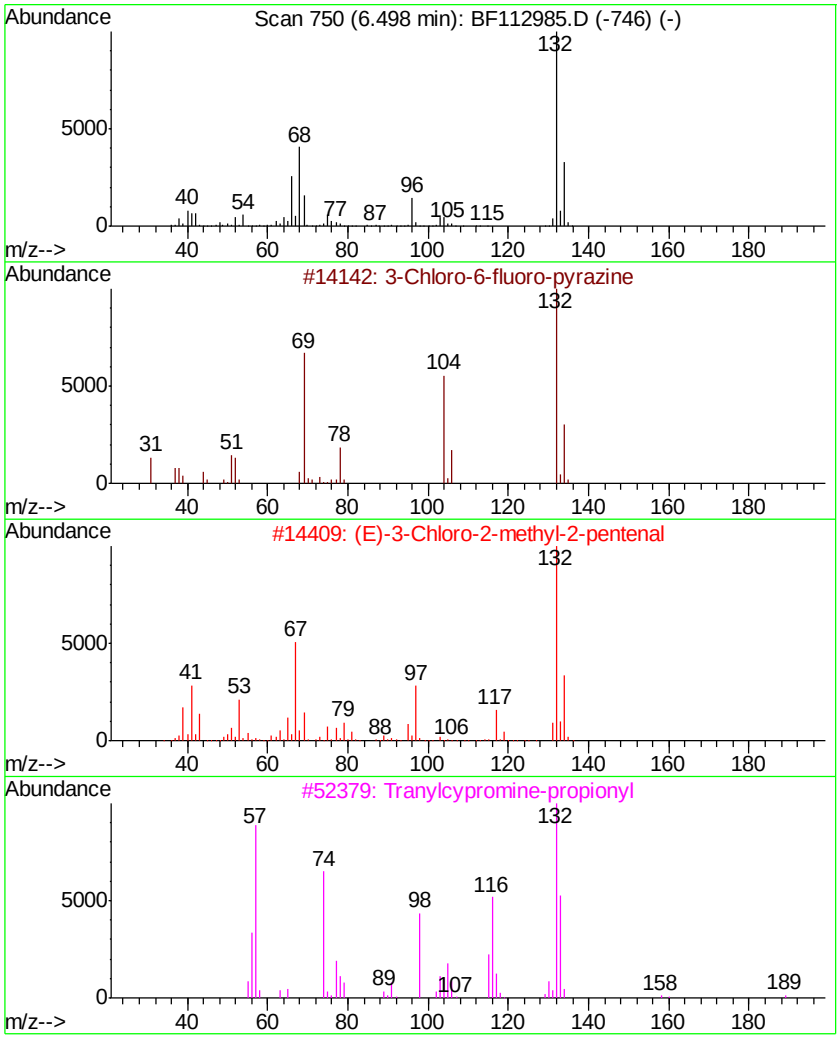
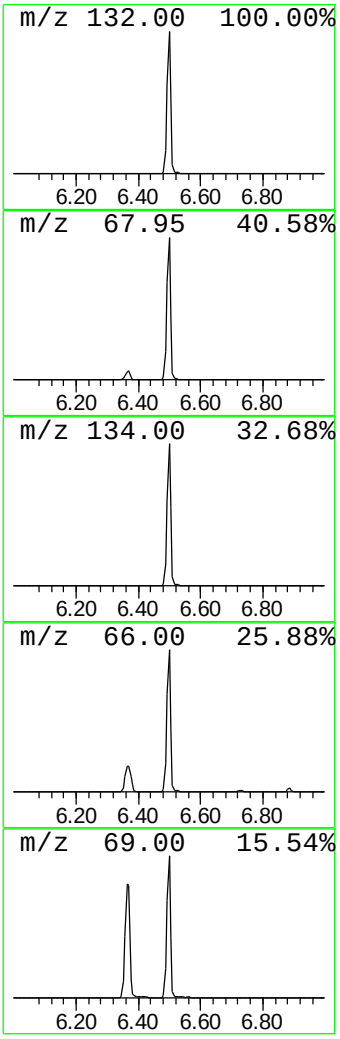
Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	64.85 ng	2557430	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Amphetaminil	250	C17H18N2	017590-01-1	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112985.D
Acq On : 12 Mar 2019 5:44
Operator : JU/SJ
Sample : K1817-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-027-B112-030719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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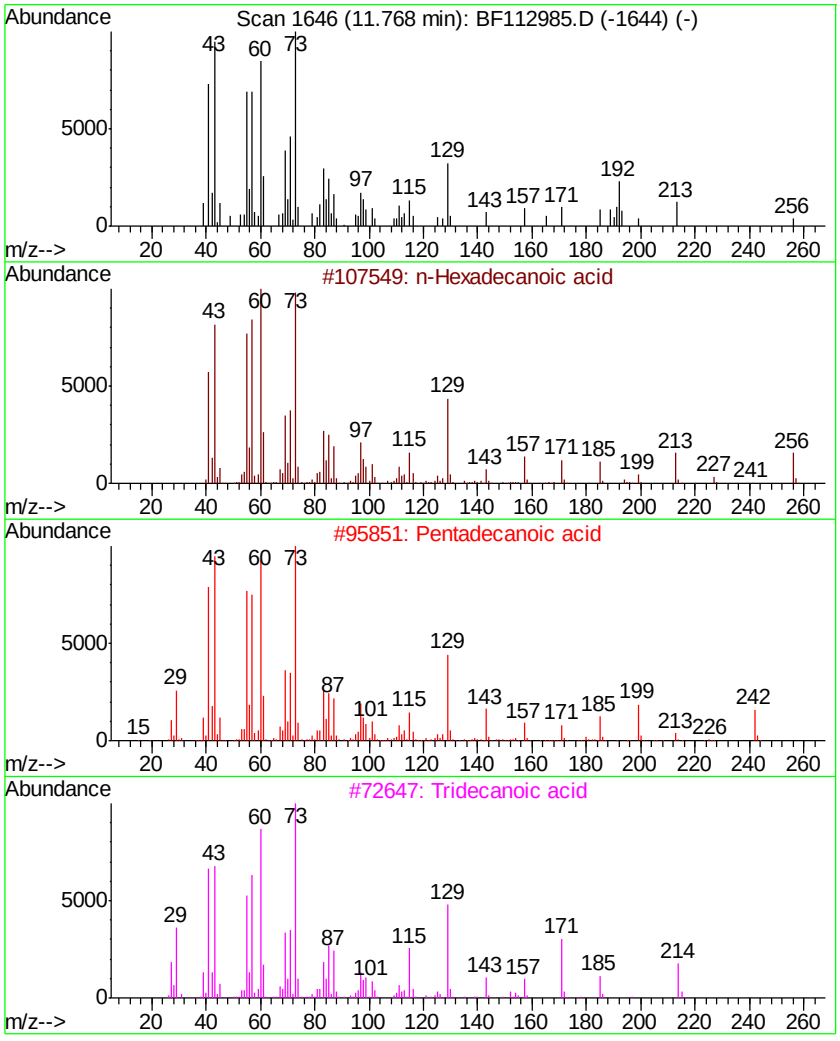
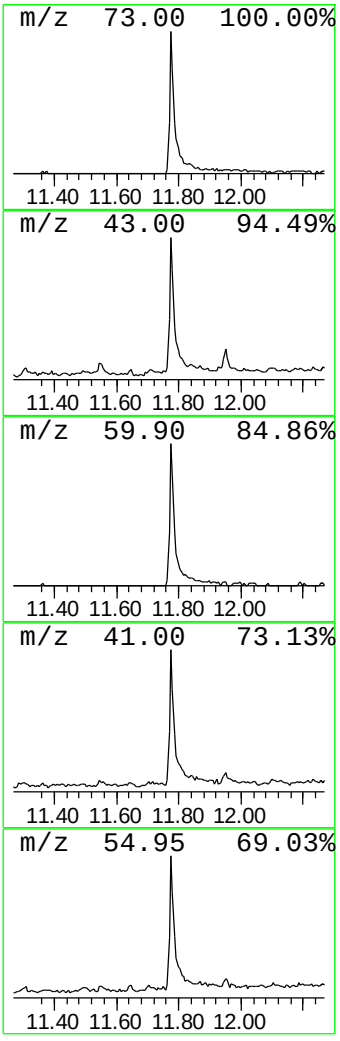
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	4.49 ng	311918	Phenanthrene-d10	11.24

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	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	25





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112985.D
Acq On : 12 Mar 2019 5:44
Operator : JU/SJ
Sample : K1817-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-027-B112-030719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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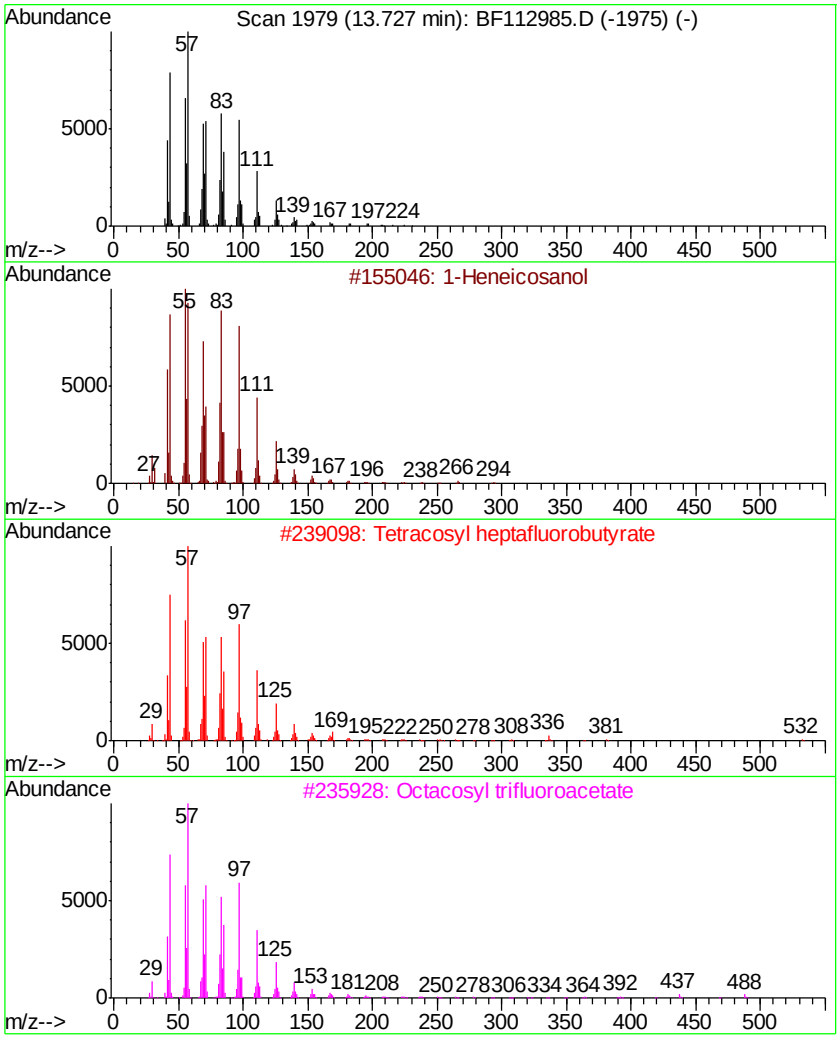
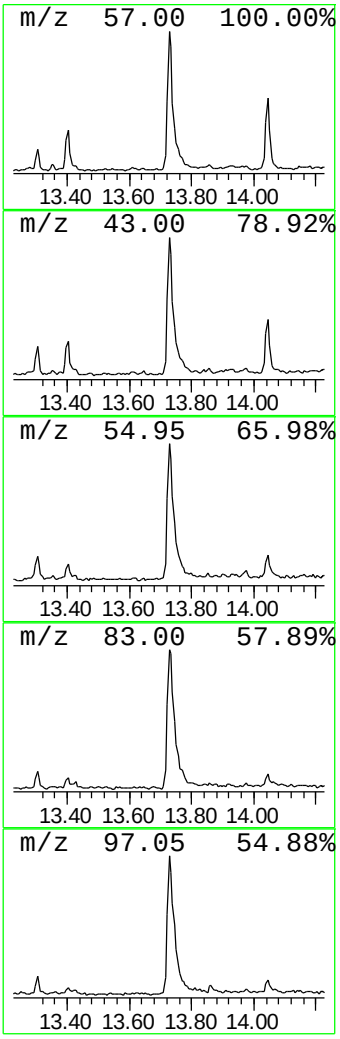
Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	7.66 ng	493545	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
3	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
4	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112985.D
Acq On : 12 Mar 2019 5:44
Operator : JU/SJ
Sample : K1817-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-027-B112-030719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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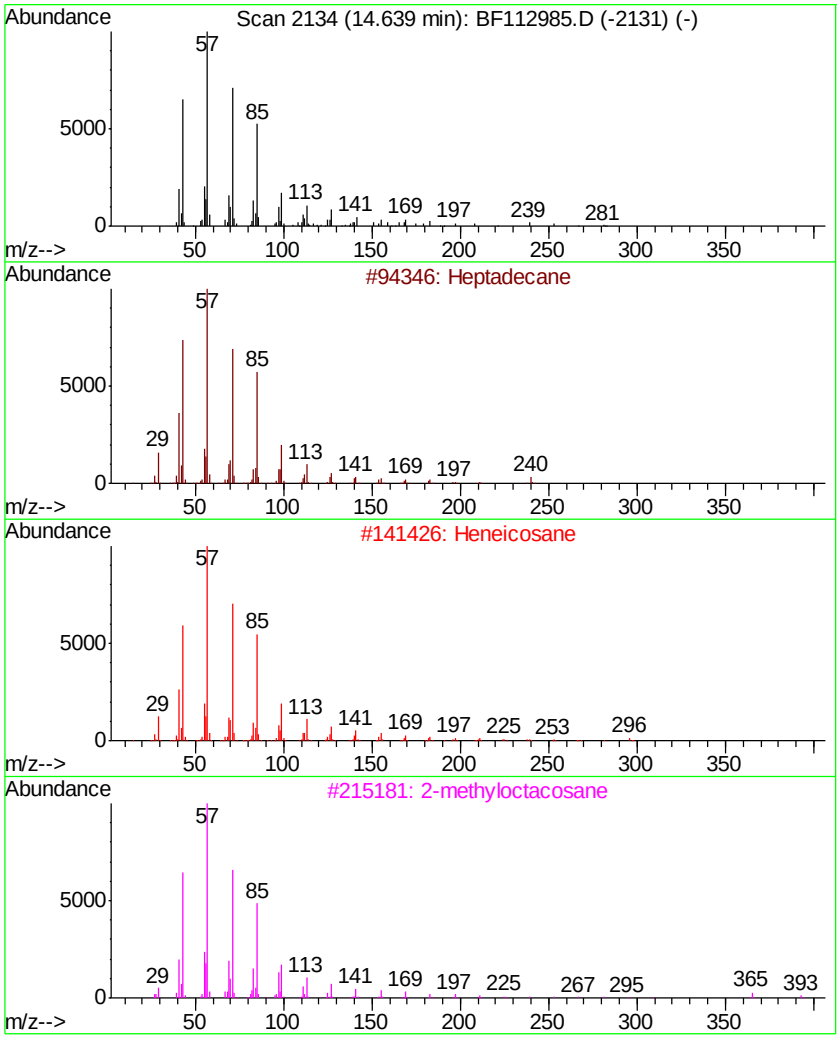
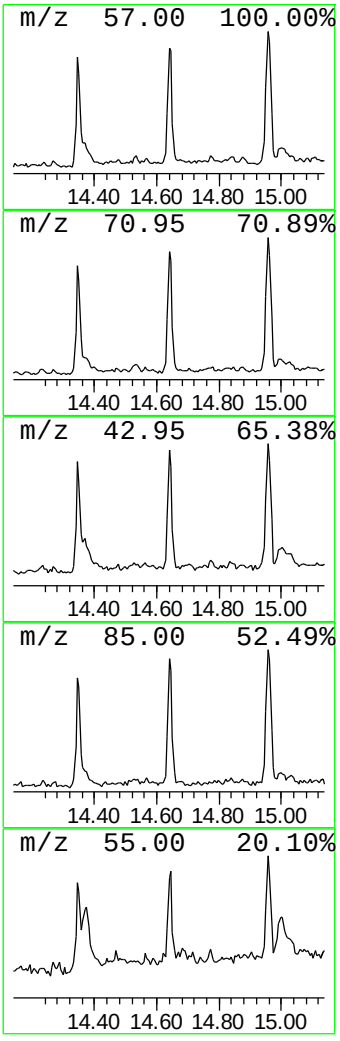
Peak Number 5 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.55 ng	119997	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	2-Bromotetradecane	276	C14H29Br	074036-95-6	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Library Search Compound Report

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Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : PST-027-B112-030719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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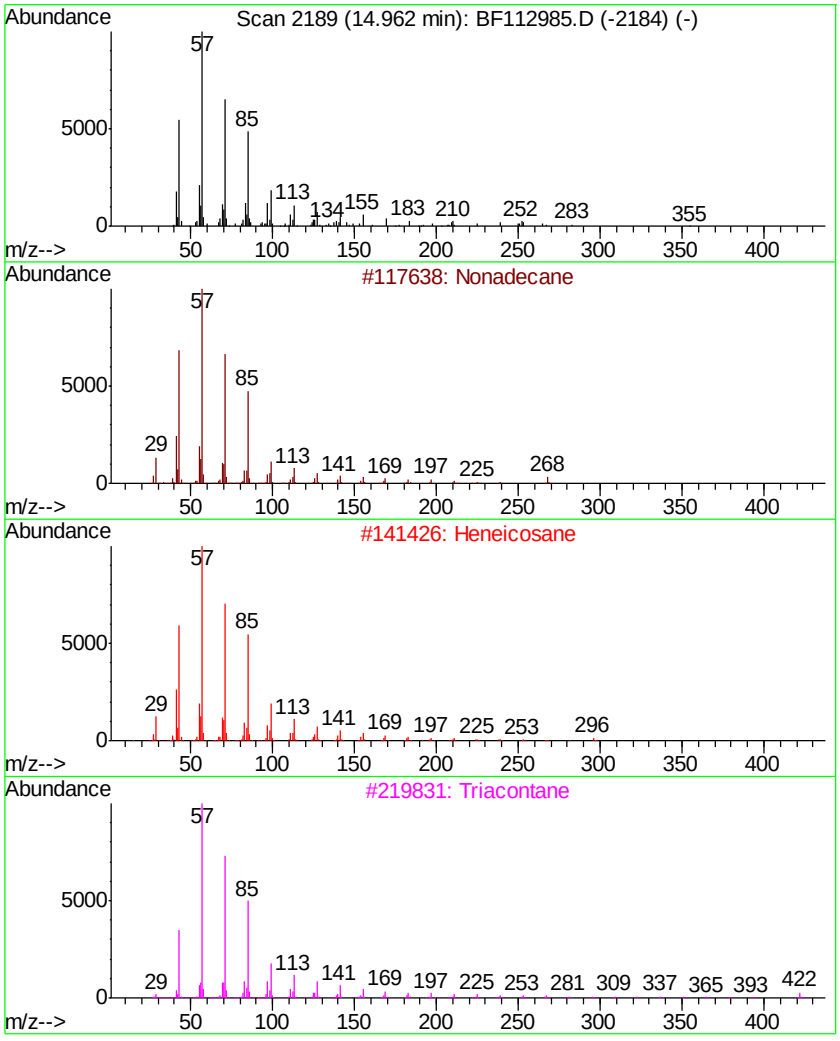
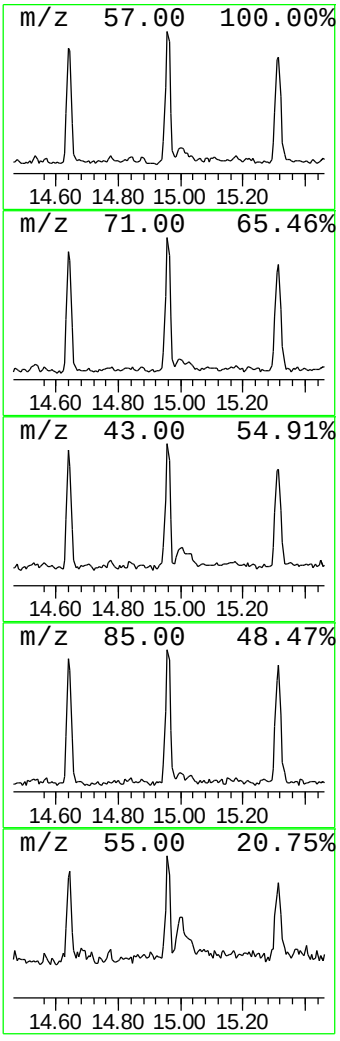
Peak Number 6 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	3.04 ng	142834	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Triacontane	422	C30H62	000638-68-6	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87





Library Search Compound Report

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Acq On : 12 Mar 2019 5:44
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Sample : K1817-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-027-B112-030719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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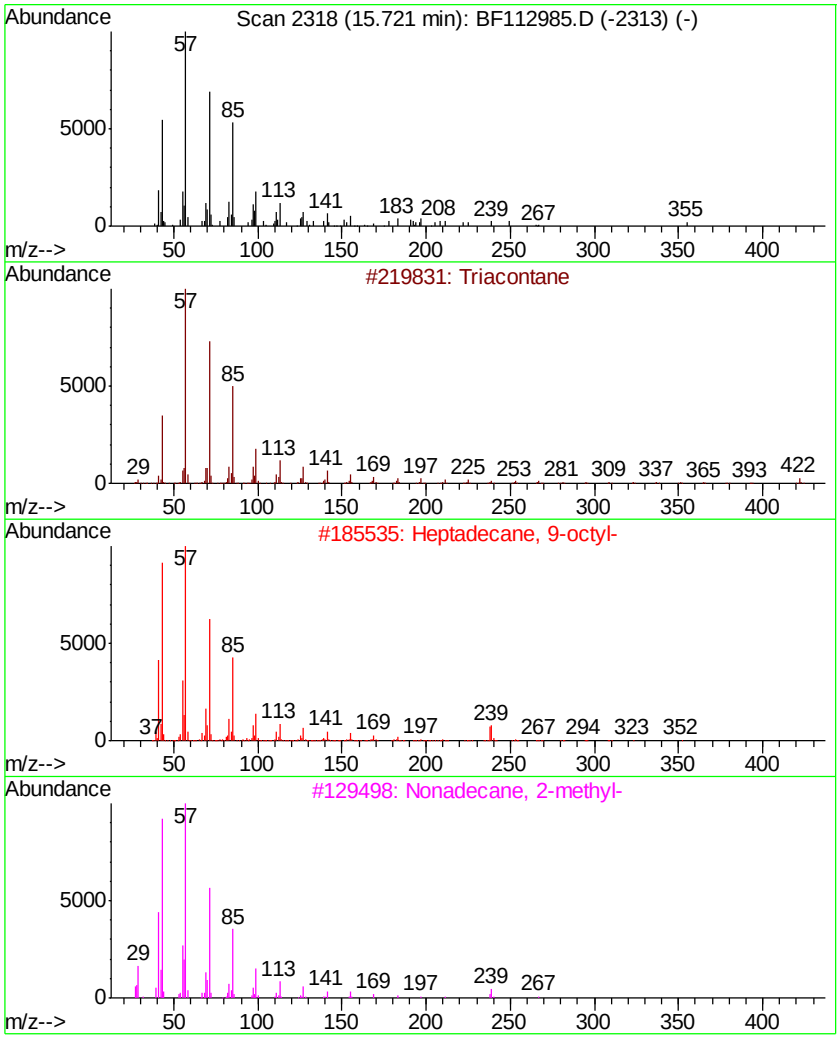
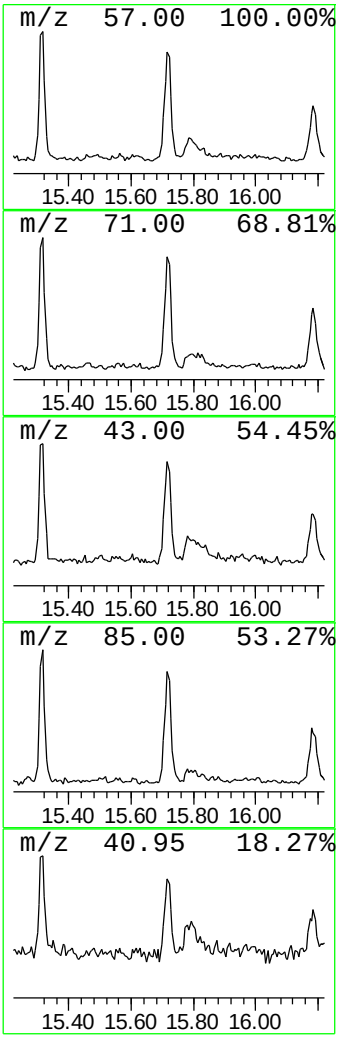
Peak Number 7 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	2.95 ng	138488	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heneicosane	296	C21H44	000629-94-7	90





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Data File : BF112985.D
Acq On : 12 Mar 2019 5:44
Operator : JU/SJ
Sample : K1817-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PST-027-B112-030719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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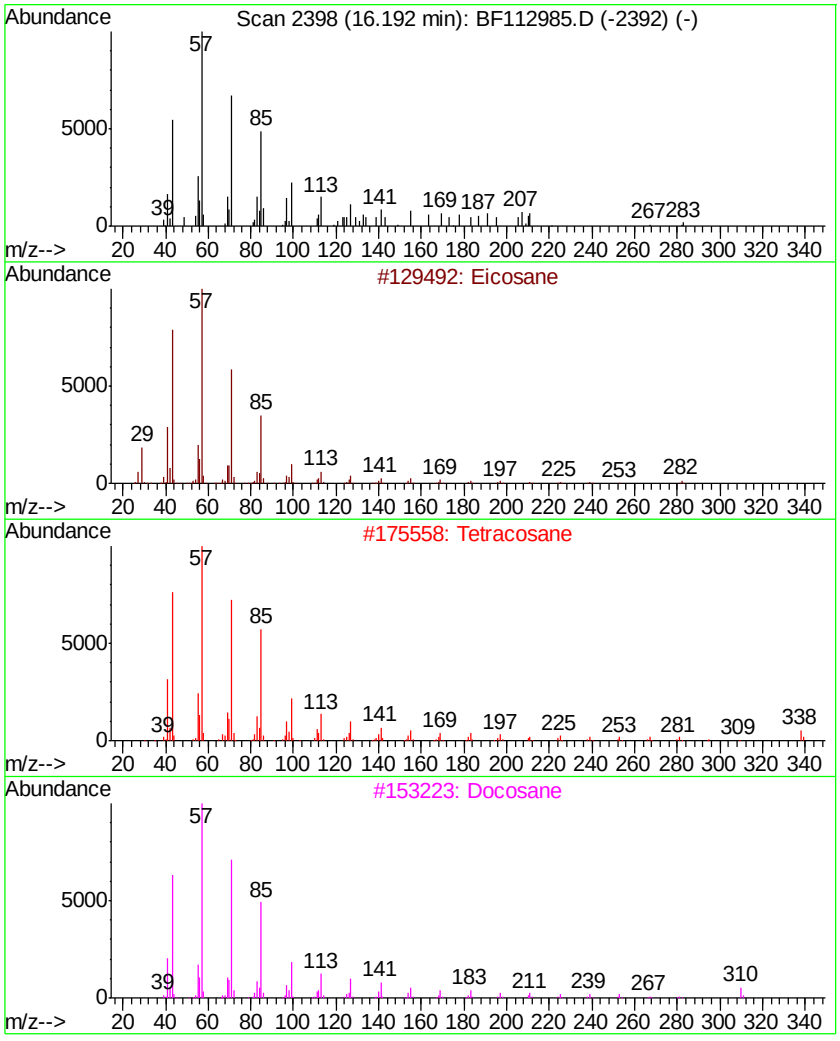
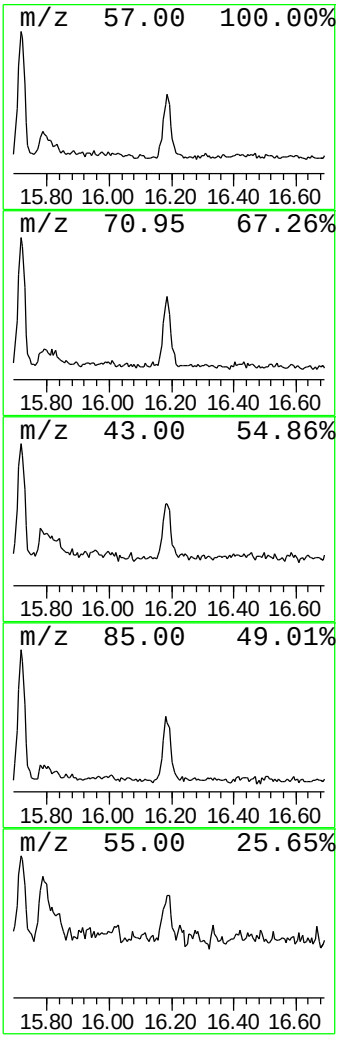
Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.20 ng	103392	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Docosane	310	C22H46	000629-97-0	90
4	Pentacosane	352	C25H52	000629-99-2	90
5	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031119\
Data File : BF112985.D
Acq On : 12 Mar 2019 5:44
Operator : JU/SJ
Sample : K1817-04
Misc :
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Instrument : BNA_F
ClientSampleId : PST-027-B112-030719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
unknown6.50	6.50	64.8	ng	2557430	1	6.73	788662	20.0
n-Hexadecanoic acid	11.77	4.5	ng	311918	4	11.24	1390340	20.0
1-Heneicosanol	13.73	7.7	ng	493545	5	13.86	1288840	20.0
Heptadecane	14.64	2.5	ng	119997	6	15.27	940046	20.0
Nonadecane	14.96	3.0	ng	142834	6	15.27	940046	20.0
Triacontane	15.72	3.0	ng	138488	6	15.27	940046	20.0
Eicosane	16.19	2.2	ng	103392	6	15.27	940046	20.0