LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022719\
Data File : BF112721.D
Acq On : 27 Feb 2019 16:10
Operator : JU/SJ
Sample : K1613-03 5X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : L-1

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	556	rBV	1042738	900356	36.44%	3.874%
2	6.357	722	726	731	rBV	1236548	976312	39.51%	4.200%
3	6.498	746	750	754	rBV	1139603	962981	38.97%	4.143%
4	6.739	787	791	794	rBV	1465630	1207689	48.87%	5.196%
5	6.892	814	817	820	rBV	924667	705975	28.57%	3.037%
6	7.292	881	885	888	rBV	651513	546761	22.13%	2.352%
7	8.016	1005	1008	1012	rBV	1797952	1557491	63.03%	6.701%
8	9.092	1187	1191	1194	rVB	1268296	937803	37.95%	4.035%
9	9.486	1255	1258	1261	rBV	55471	45339	1.83%	0.195%
10	9.769	1302	1306	1309	rBV	1813748	1620620	65.58%	6.972%
11	10.545	1434	1438	1441	rBV	574066	469915	19.02%	2.022%
12	11.239	1553	1556	1560	rBV	1742648	1508044	61.03%	6.488%
13	11.786	1641	1649	1671	rVV	675845	1229361	49.75%	5.289%
14	12.445	1757	1761	1763	rBV2	75989	77656	3.14%	0.334%
15	12.486	1763	1768	1774	rVV7	68465	184429	7.46%	0.793%
16	12.568	1775	1782	1795	rVV	1613561	2471057	100.00%	10.631%
17	12.668	1797	1799	1805	rVB	80329	90516	3.66%	0.389%
18	12.821	1821	1825	1828	rBV	838634	697117	28.21%	2.999%
19	12.927	1840	1843	1847	rVB	112284	89568	3.62%	0.385%
20	13.298	1903	1906	1909	rBV	90597	81305	3.29%	0.350%
21	13.739	1976	1981	1984	rVB2	55811	85206	3.45%	0.367%
22	13.862	1998	2002	2006	rBV2	1878389	1796795	72.71%	7.730%
23	14.057	2032	2035	2040	rBV	98558	110378	4.47%	0.475%
24	14.362	2083	2087	2091	rVB	177866	177593	7.19%	0.764%
25	14.657	2133	2137	2141	rBV	411743	507476	20.54%	2.183%
26	14.868	2170	2173	2176	rBV	33422	46264	1.87%	0.199%
27	14.974	2187	2191	2196	rBV	534332	565633	22.89%	2.434%
28	15.151	2218	2221	2223	rBV	25176	29631	1.20%	0.127%
29	15.204	2227	2230	2235	rVV2	55023	92161	3.73%	0.397%
30	15.268	2236	2241	2246	rVV	1294237	1520741	61.54%	6.543%
31	15.333	2247	2252	2258	rVB	583054	748183	30.28%	3.219%
32	15.739	2315	2321	2326	rBV	473140	681010	27.56%	2.930%
33	16.209	2395	2401	2409	rVB	226786	398968	16.15%	1.716%
34	16.756	2490	2494	2500	rVB2	64371	122868	4.97%	0.529%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022719\
Data File : BF112721.D
Acq On : 27 Feb 2019 16:10
Operator : JU/SJ
Sample : K1613-03 5X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
L-1

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: 23243202

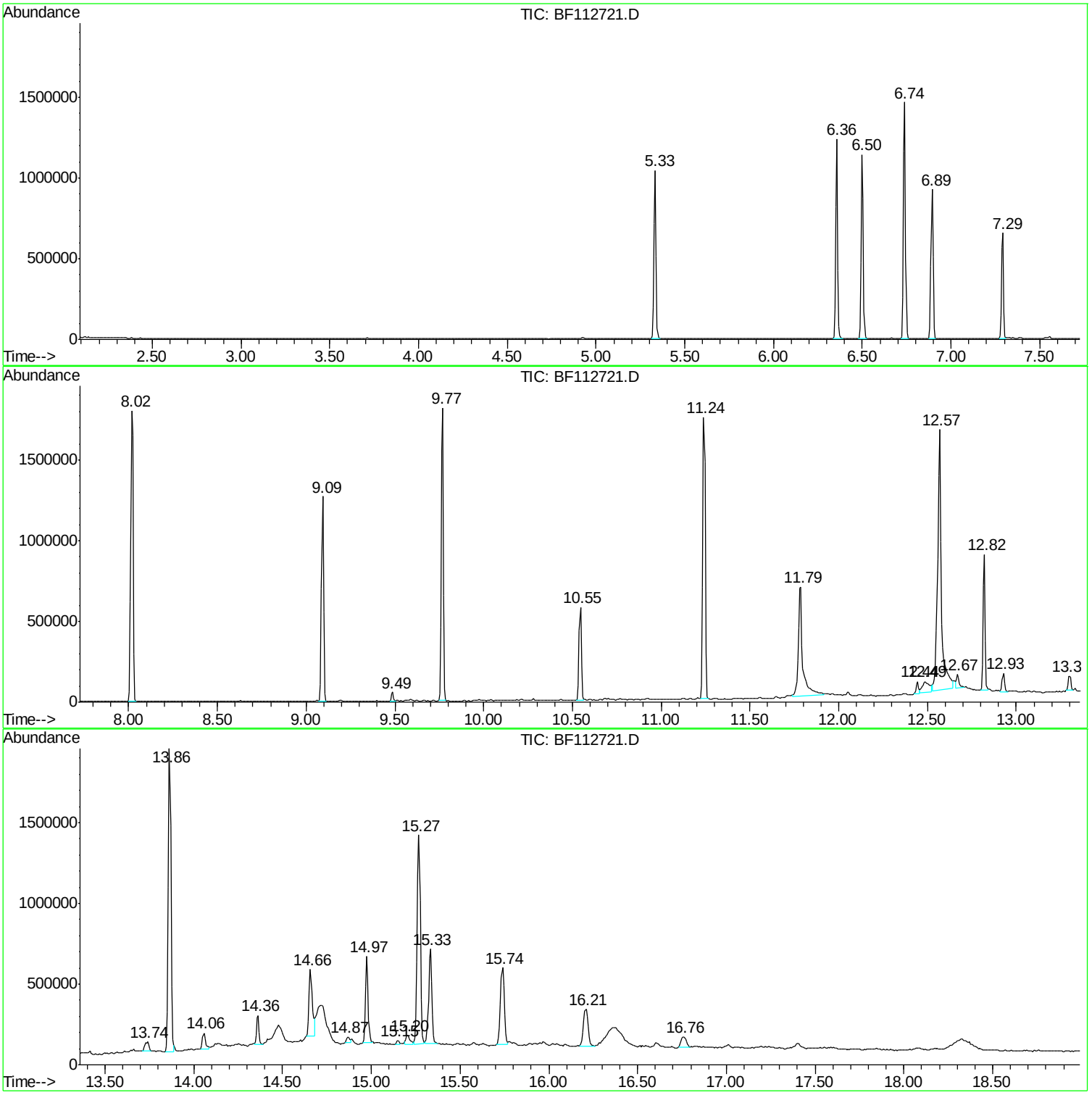
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022719\
Data File : BF112721.D
Acq On : 27 Feb 2019 16:10
Operator : JU/SJ
Sample : K1613-03 5X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : L-1

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\BF022719\
Data File : BF112721.D
Acq On : 27 Feb 2019 16:10
Operator : JU/SJ
Sample : K1613-03 5X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : L-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

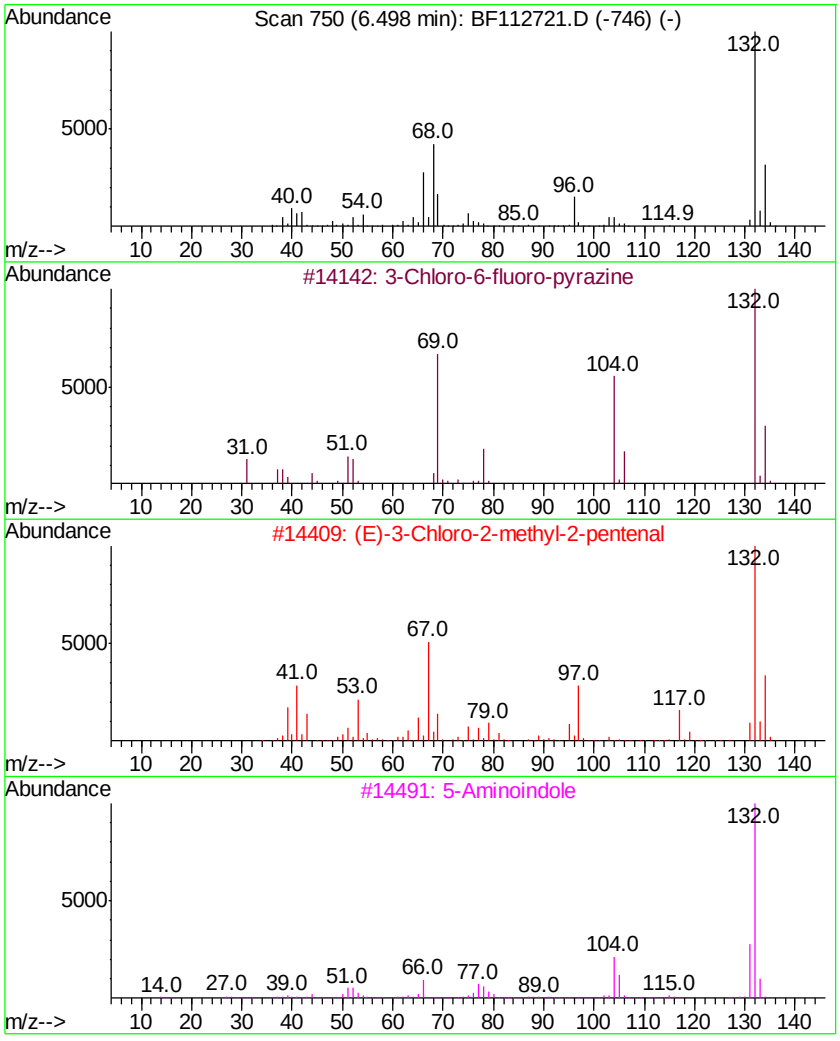
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

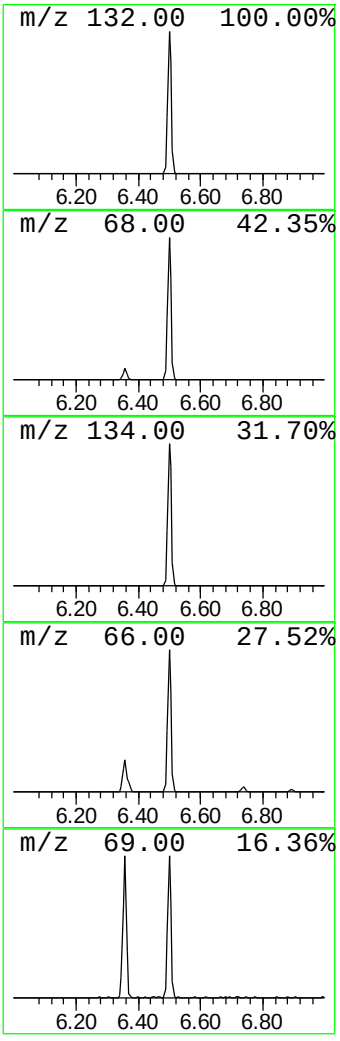
****

Peak Number 1 unknown6.50 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	15.95 ng	962981	1,4-Dichlorobenzene-d4	6.74

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	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	10
4	Amphetaminil	250	C17H18N2	017590-01-1	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022719\
Data File : BF112721.D
Acq On : 27 Feb 2019 16:10
Operator : JU/SJ
Sample : K1613-03 5X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : L-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

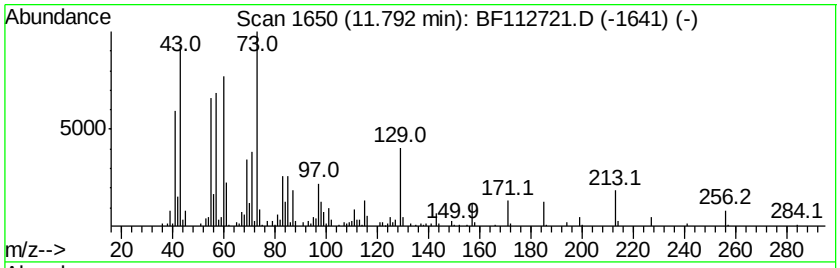
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

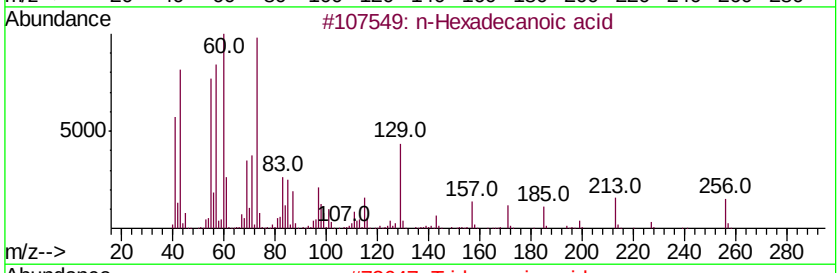
****

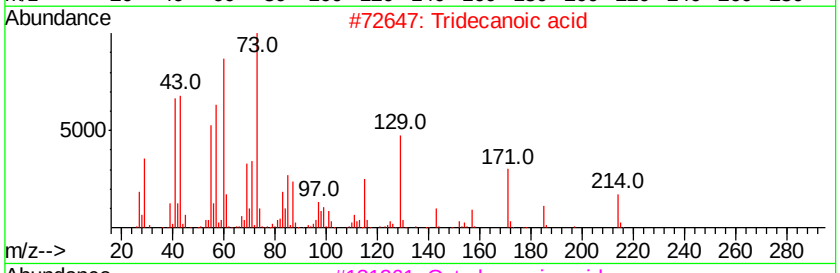
Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

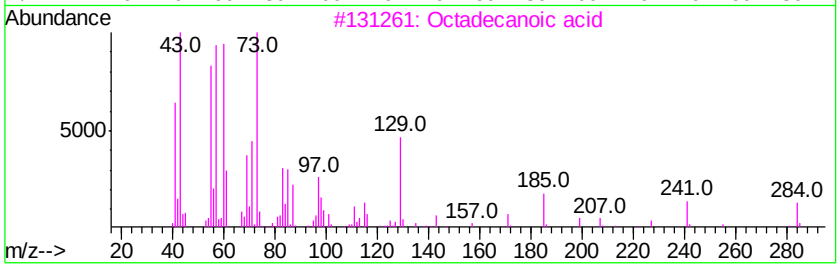
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	16.30 ng	1229360	Phenanthrene-d10	11.24

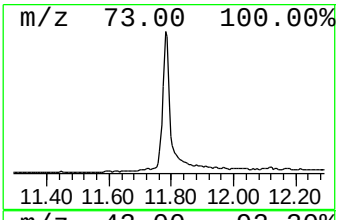
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Octadecanoic acid	284	C18H36O2	000057-11-4	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	68

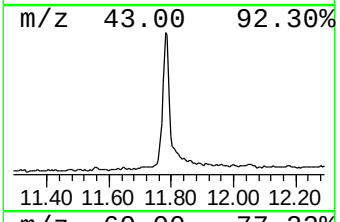


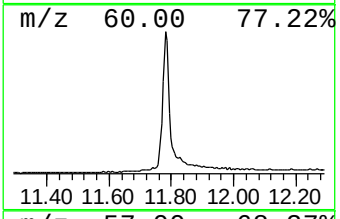


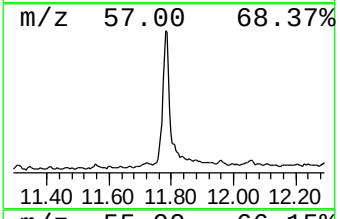


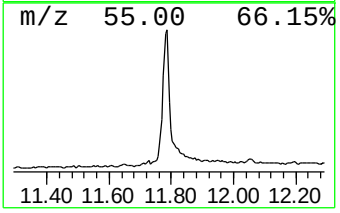












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022719\
Data File : BF112721.D
Acq On : 27 Feb 2019 16:10
Operator : JU/SJ
Sample : K1613-03 5X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : L-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

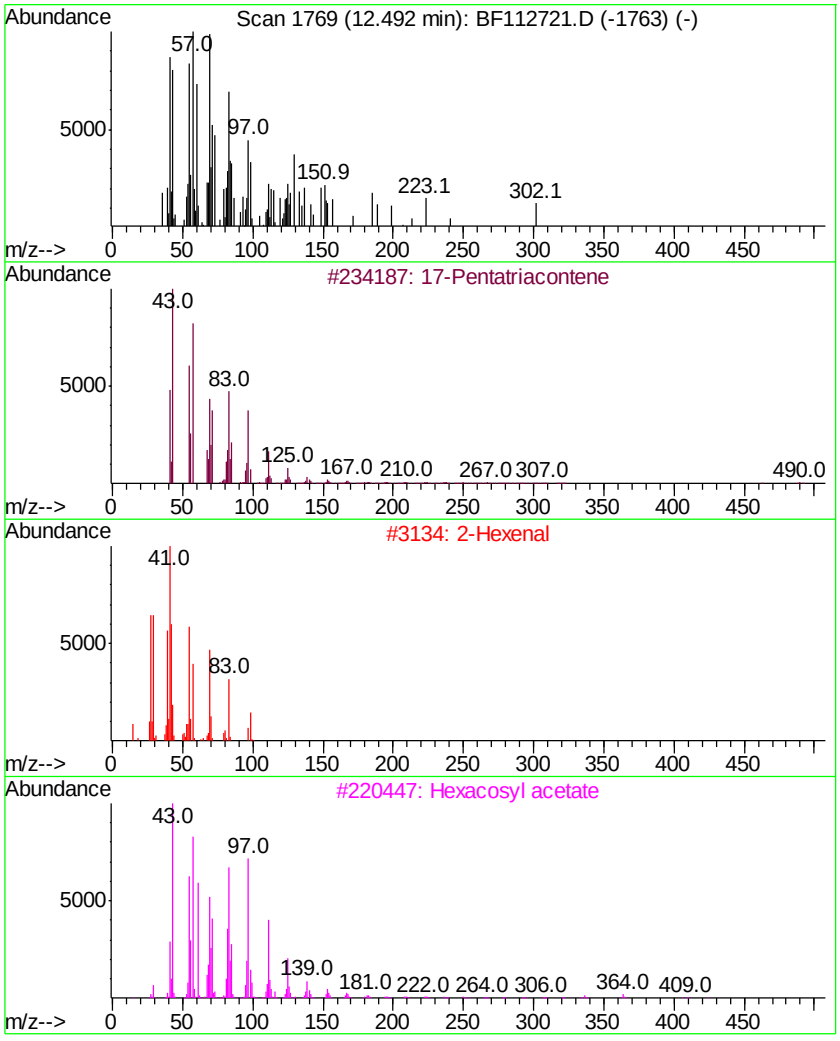
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

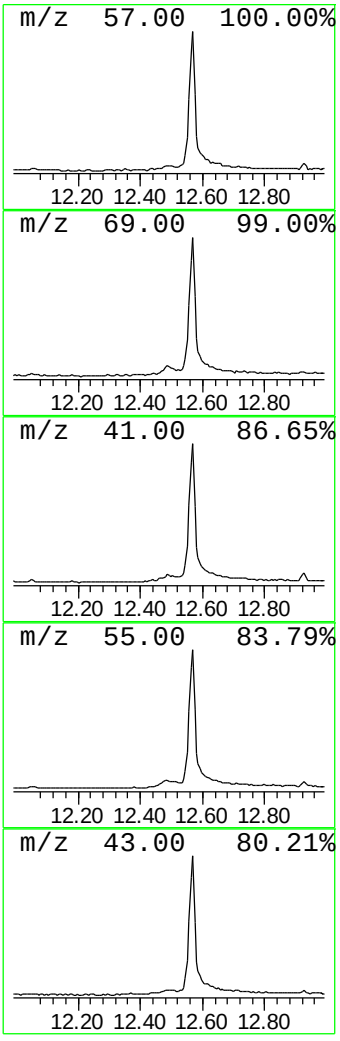
****

Peak Number 4 17-Pentatriacontene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	2.45 ng	184429	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	52
2	2-Hexenal	98	C6H10O	000505-57-7	43
3	Hexacosyl acetate	424	C28H56O2	000822-32-2	41
4	Heptacosyl acetate	438	C29H58O2	1000351-78-2	41
5	Tetracosyl acetate	396	C26H52O2	1000351-78-1	41





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022719\
Data File : BF112721.D
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Sample : K1613-03 5X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : L-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

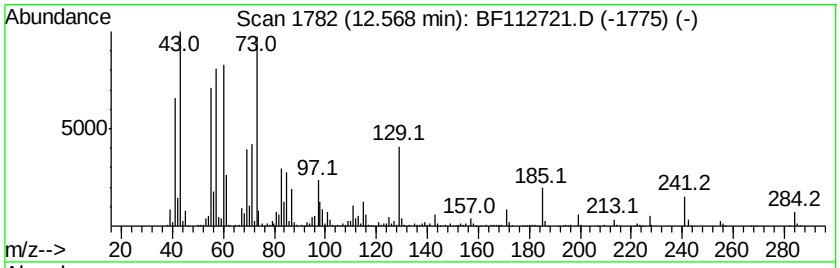
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

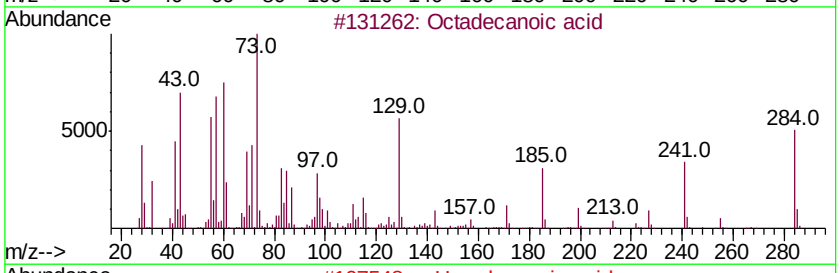
****

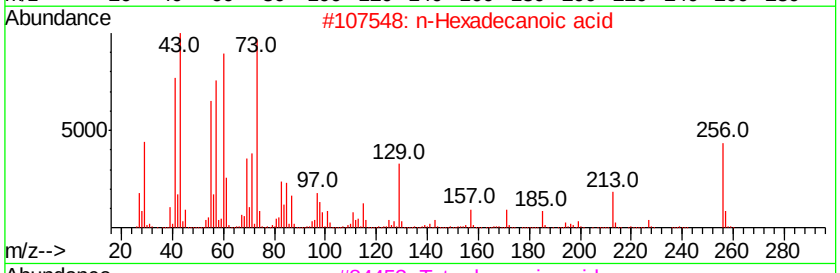
Peak Number 5 Octadecanoic acid Concentration Rank 1

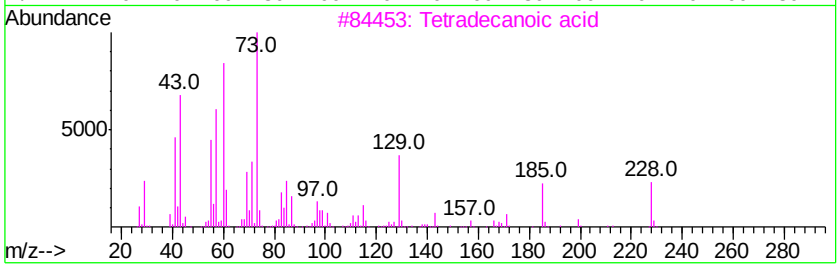
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	27.51 ng	2471060	Chrysene-d12	13.86

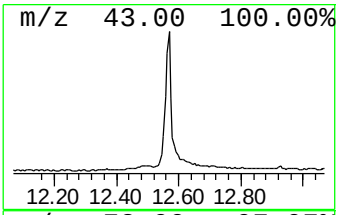
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68

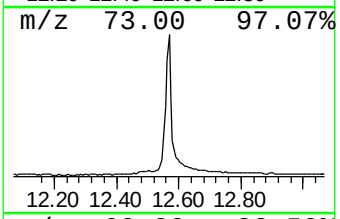


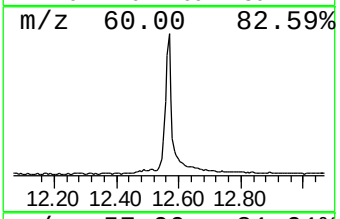


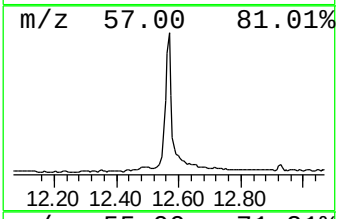


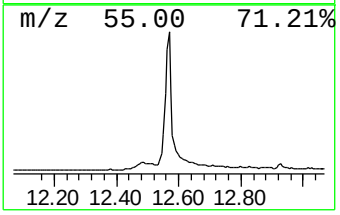












Library Search Compound Report

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Sample : K1613-03 5X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : L-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

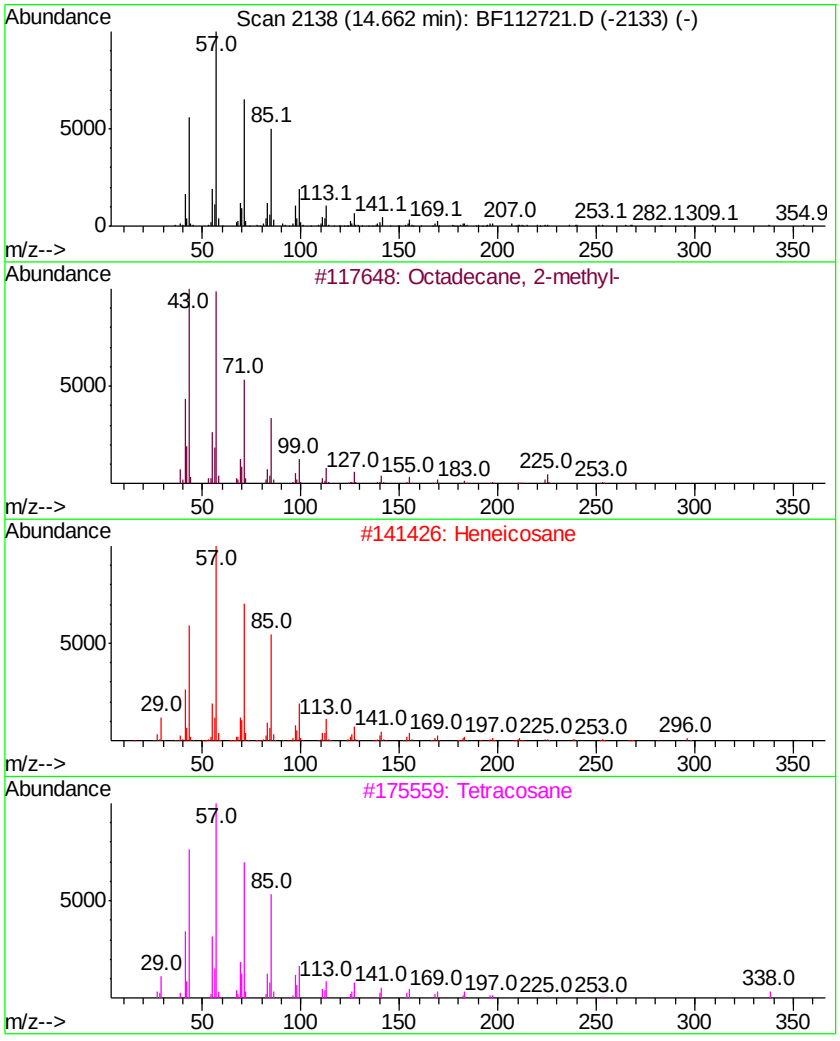
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

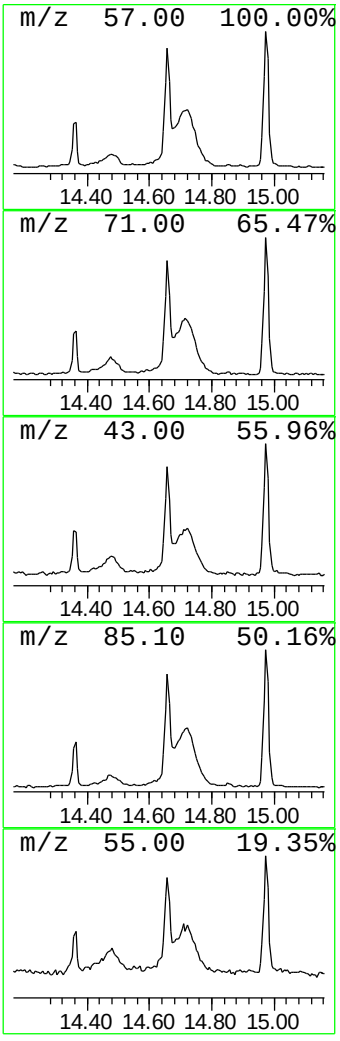
****

Peak Number 6 Octadecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	6.67 ng	507476	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Triacontane	422	C30H62	000638-68-6	91





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : L-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

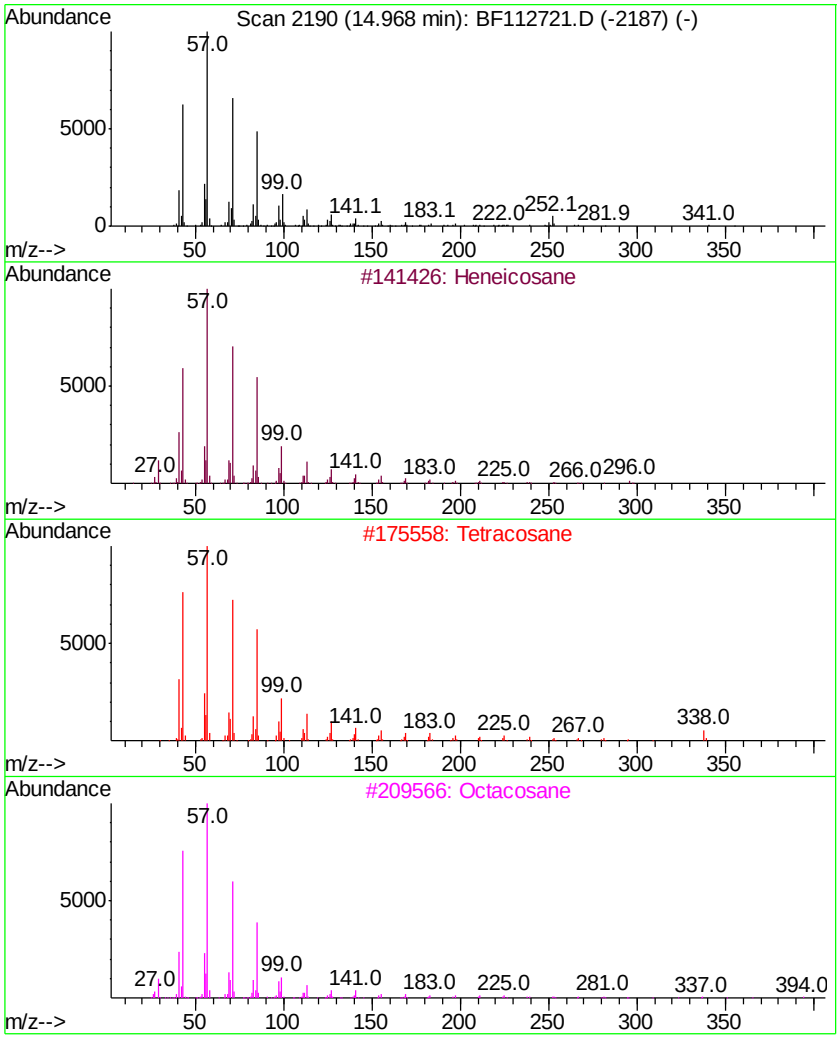
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

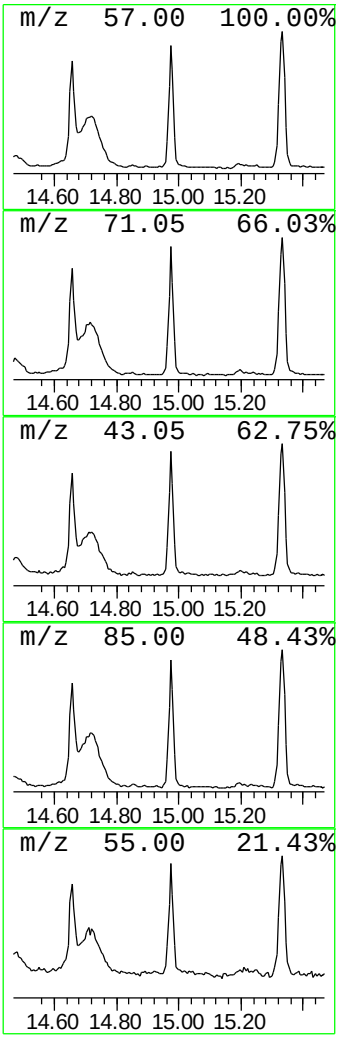
****

Peak Number 7 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	7.44 ng	565633	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tridecane, 6-propyl-	226	C16H34	055045-10-8	90
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87





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Instrument : BNA_F
ClientSampleId : L-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

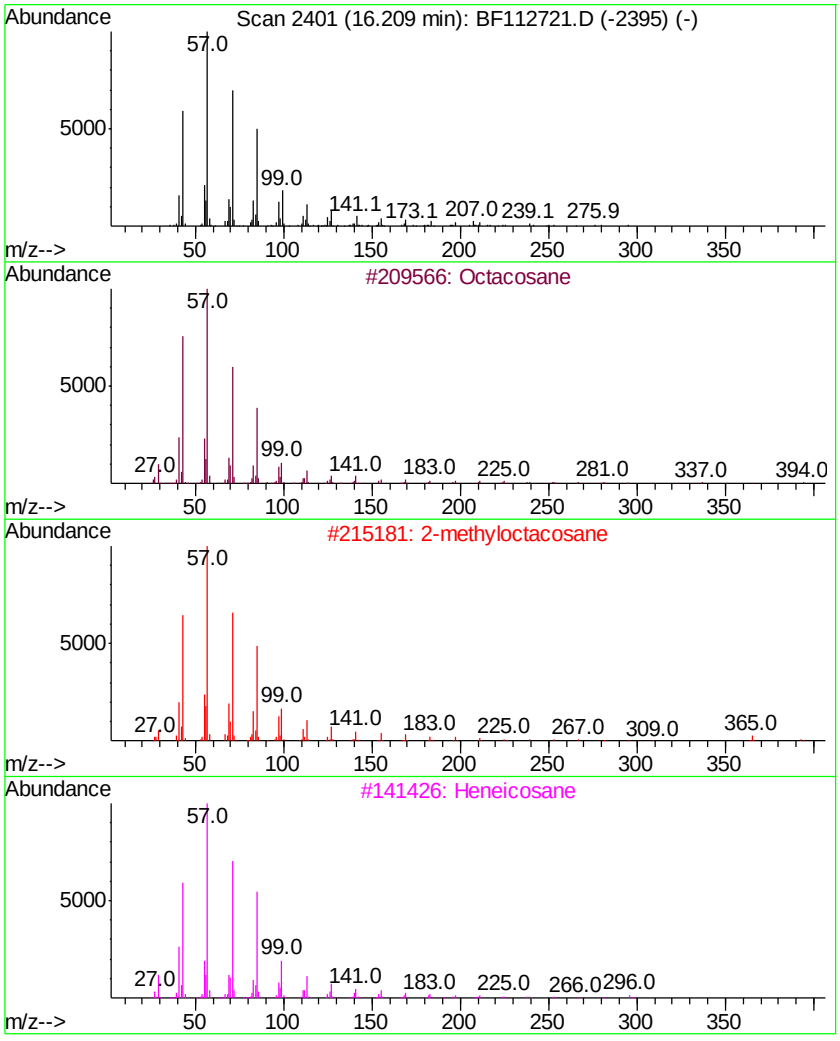
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

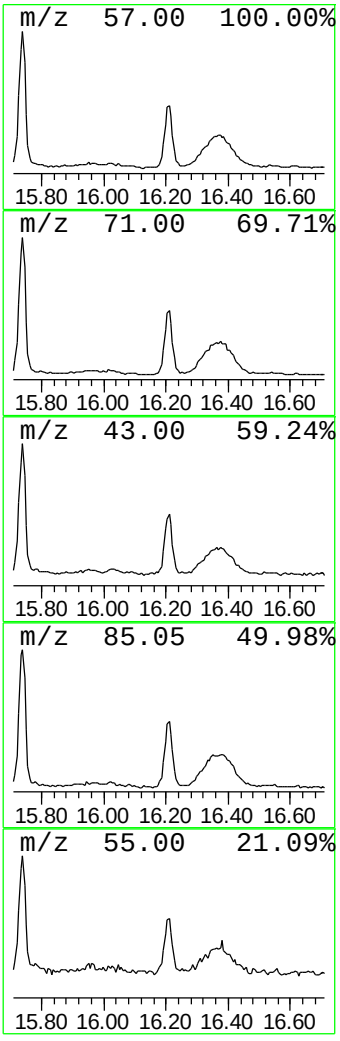
****

Peak Number 10 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	5.25 ng	398968	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Triacontane	422	C30H62	000638-68-6	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022719\
Data File : BF112721.D
Acq On : 27 Feb 2019 16:10
Operator : JU/SJ
Sample : K1613-03 5X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : L-1

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	15.9	ng	962981	1	6.74	1207690	20.0
n-Hexadecanoic acid	11.79	16.3	ng	1229360	4	11.24	1508040	20.0
17-Pentatriacontene	12.49	2.5	ng	184429	4	11.24	1508040	20.0
Octadecanoic acid	12.57	27.5	ng	2471060	5	13.86	1796800	20.0
Octadecane, 2-met...	14.66	6.7	ng	507476	6	15.27	1520740	20.0
Heneicosane	14.97	7.4	ng	565633	6	15.27	1520740	20.0
Octacosane	16.21	5.3	ng	398968	6	15.27	1520740	20.0