LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121318\
Data File : BF111379.D
Acq On : 13 Dec 2018 19:36
Operator : JU/SJ
Sample : J6214-51
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-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-BF121218.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	4.046	327	333	339	rBV2	52263	66197	1.09%	0.155%
2	4.246	347	367	369	rBV3	36175	135987	2.24%	0.318%
3	4.999	491	495	498	rBV	102303	115115	1.90%	0.269%
4	5.157	512	522	526	rBV2	33337	73668	1.21%	0.172%
5	5.410	561	565	579	rVB	3123692	3123551	51.51%	7.306%
6	6.428	734	738	749	rBV	2142590	2244885	37.02%	5.251%
7	6.563	757	761	764	rBV	5515008	5157555	85.06%	12.064%
8	6.793	796	800	808	rBV	1709967	1401063	23.11%	3.277%
9	6.857	808	811	814	rBV	72010	69961	1.15%	0.164%
10	6.951	821	827	830	rBV	5509439	4818110	79.46%	11.270%
11	7.204	863	870	877	rVB2	51052	75337	1.24%	0.176%
12	7.357	890	896	898	rBV	3761779	3893580	64.21%	9.107%
13	7.781	965	968	971	rBV	58010	63431	1.05%	0.148%
14	7.863	977	982	990	rVB2	43785	70900	1.17%	0.166%
15	8.075	1014	1018	1020	rBV	2045967	1662887	27.42%	3.890%
16	8.092	1020	1021	1025	rVB	226748	184291	3.04%	0.431%
17	8.316	1055	1059	1063	rBV	61399	80844	1.33%	0.189%
18	9.151	1197	1201	1205	rBV	6480692	6063768	100.00%	14.184%
19	9.539	1264	1267	1270	rBV	181850	153150	2.53%	0.358%
20	9.828	1312	1316	1319	rBV2	1821417	1577219	26.01%	3.689%
21	9.857	1319	1321	1325	rVB2	357392	306834	5.06%	0.718%
22	10.034	1348	1351	1354	rBV3	59565	63583	1.05%	0.149%
23	10.616	1446	1450	1453	rBV	3102861	2663051	43.92%	6.229%
24	10.739	1468	1471	1478	rVB6	52692	61936	1.02%	0.145%
25	11.057	1523	1525	1530	rVB	61468	66583	1.10%	0.156%
26	11.310	1565	1568	1571	rBV	1363495	1188972	19.61%	2.781%
27	11.851	1656	1660	1667	rBV	877517	925332	15.26%	2.164%
28	12.522	1771	1774	1778	rBV	79734	126629	2.09%	0.296%
29	12.633	1790	1793	1802	rVB	581923	537268	8.86%	1.257%
30	12.898	1834	1838	1841	rBV	4249956	3719423	61.34%	8.700%
31	13.804	1989	1992	1998	rVB	419275	407910	6.73%	0.954%
32	13.945	2013	2016	2020	rBV	1046228	955818	15.76%	2.236%
33	15.386	2257	2261	2266	rBV	592303	696528	11.49%	1.629%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121318\
Data File : BF111379.D
Acq On : 13 Dec 2018 19:36
Operator : JU/SJ
Sample : J6214-51
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-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-BF121218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 42751366

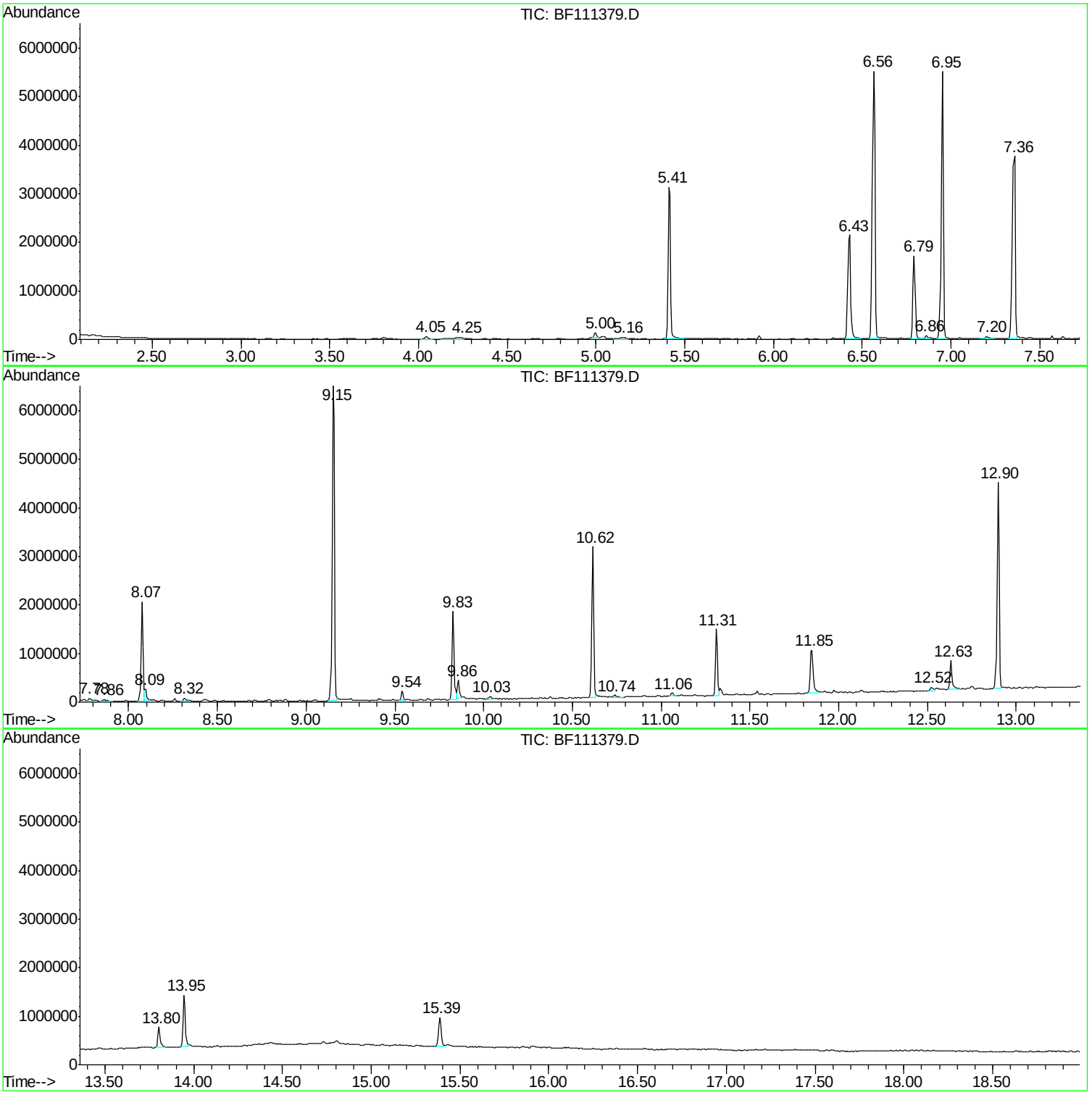
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121318\
Data File : BF111379.D
Acq On : 13 Dec 2018 19:36
Operator : JU/SJ
Sample : J6214-51
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.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\BF121318\
Data File : BF111379.D
Acq On : 13 Dec 2018 19:36
Operator : JU/SJ
Sample : J6214-51
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

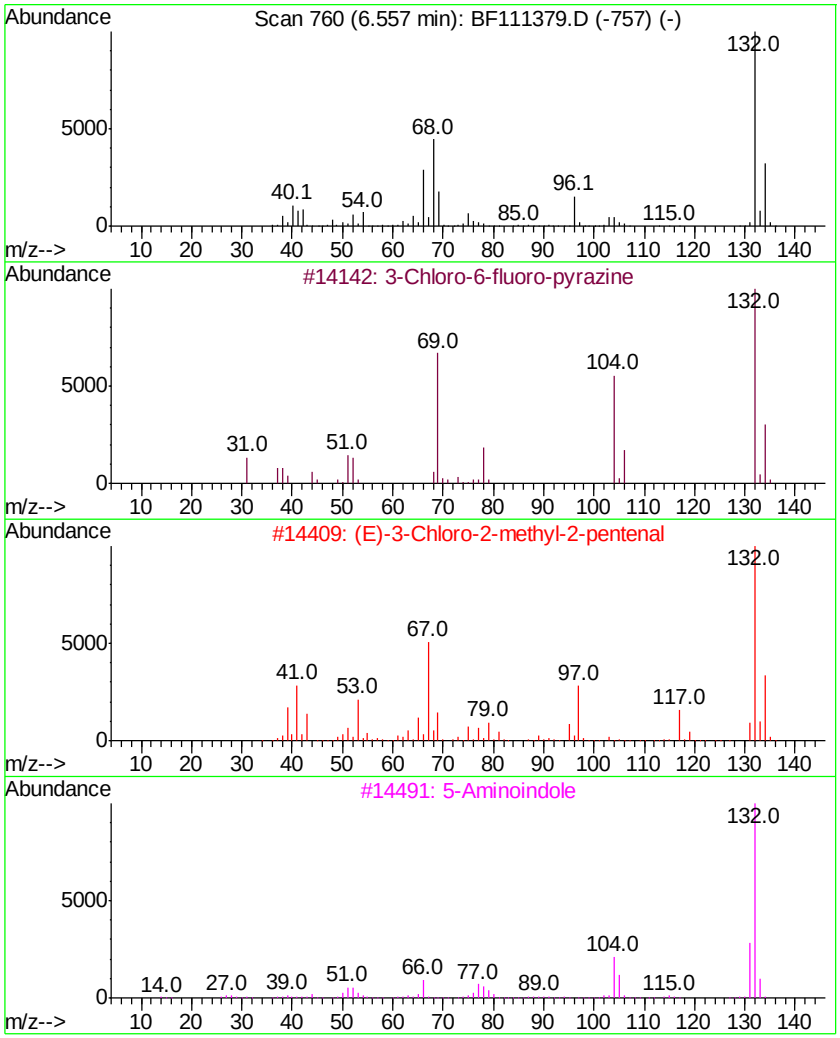
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

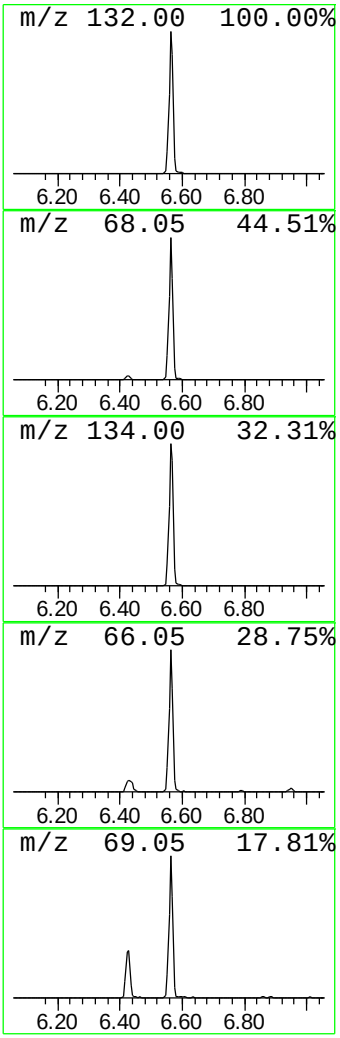
****

Peak Number 1 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	73.62 ng	5157560	1,4-Dichlorobenzene-d4	6.79

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	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121318\
Data File : BF111379.D
Acq On : 13 Dec 2018 19:36
Operator : JU/SJ
Sample : J6214-51
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

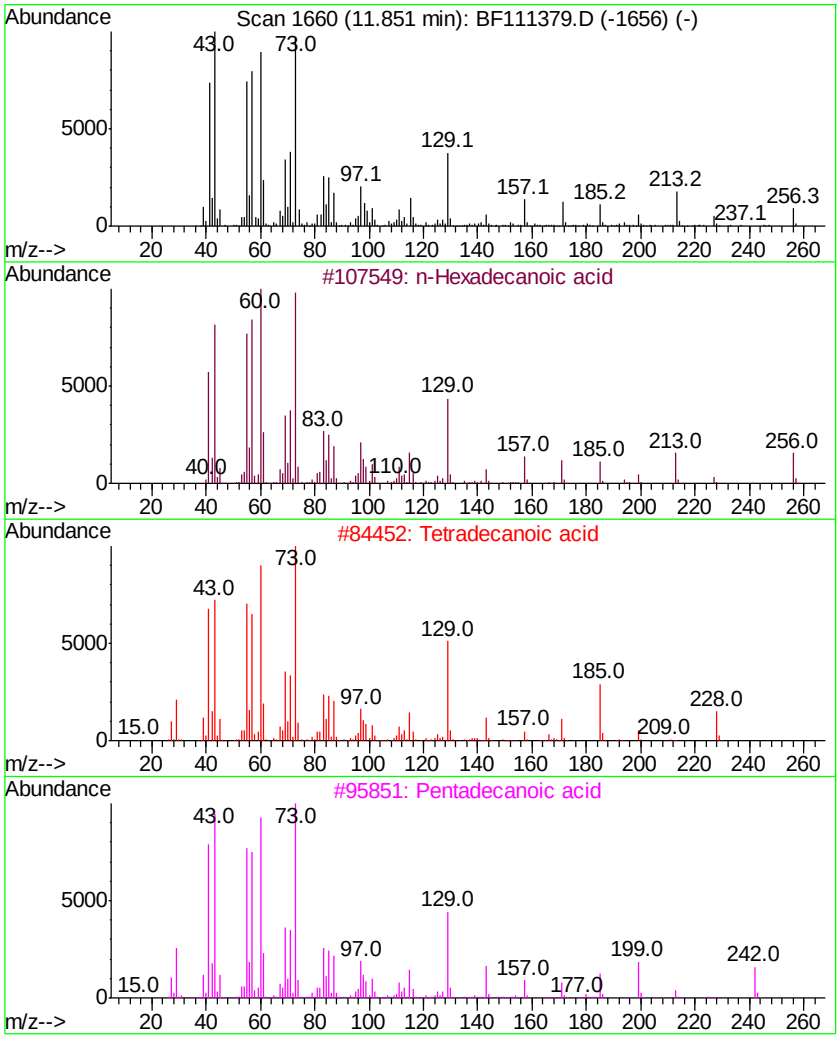
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

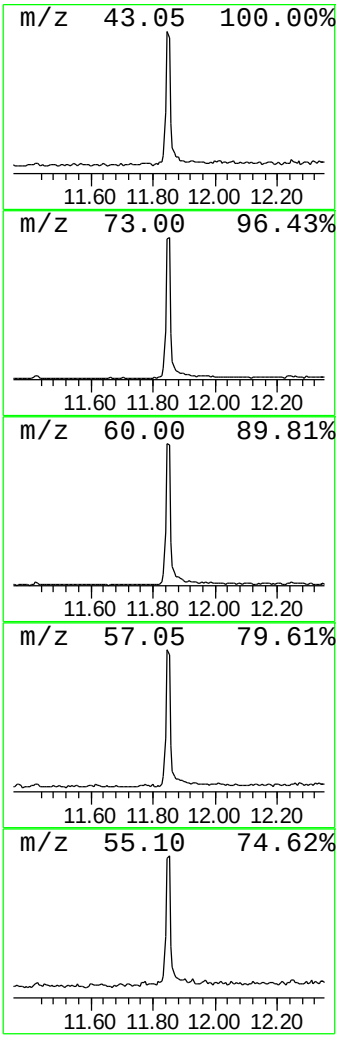
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	15.57 ng	925332	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121318\
Data File : BF111379.D
Acq On : 13 Dec 2018 19:36
Operator : JU/SJ
Sample : J6214-51
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

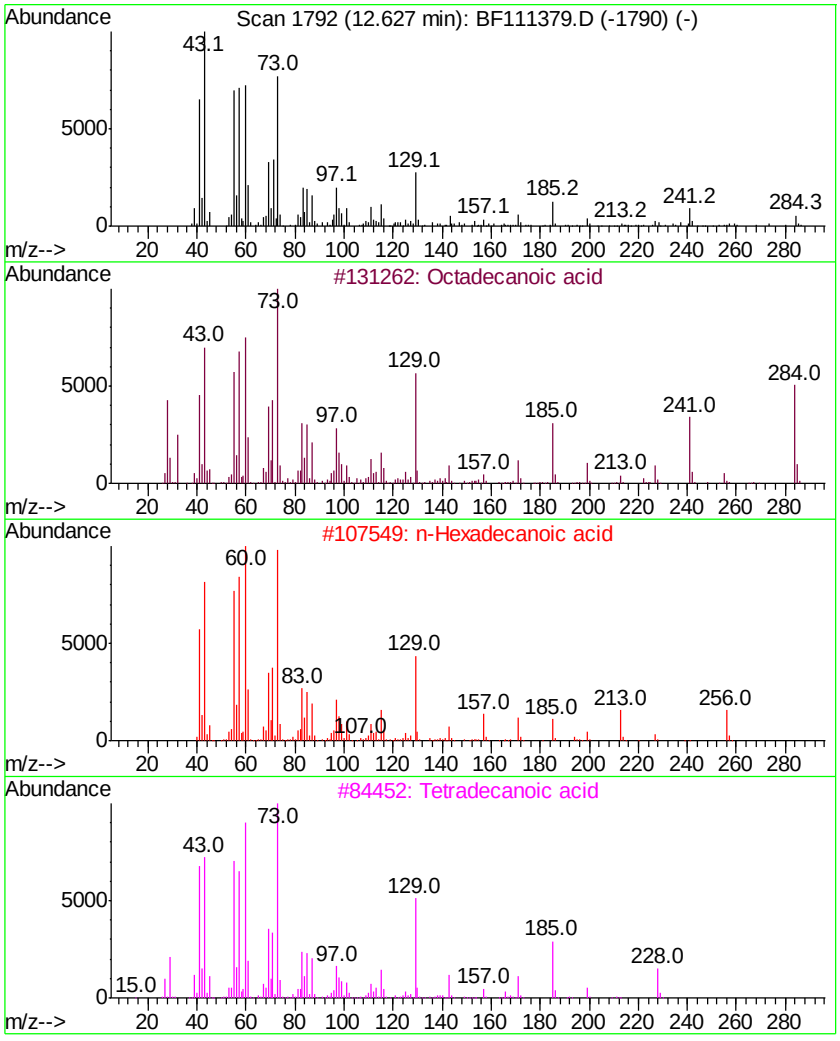
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

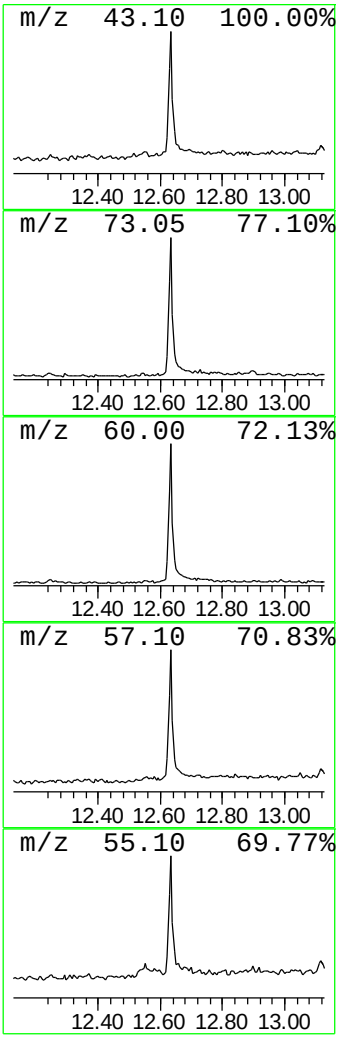
****

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	11.24 ng	537268	Chrysene-d12	13.95

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	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Tridecanoic acid	214	C13H26O2	000638-53-9	70





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121318\
Data File : BF111379.D
Acq On : 13 Dec 2018 19:36
Operator : JU/SJ
Sample : J6214-51
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

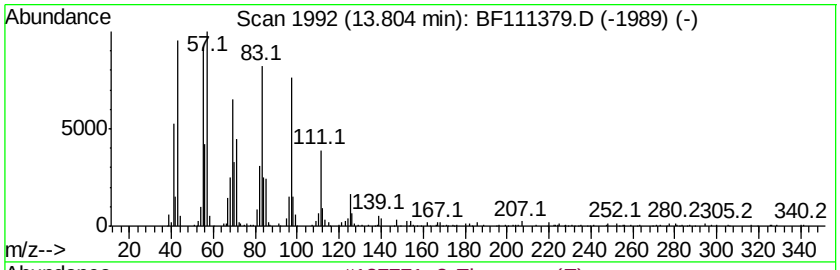
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

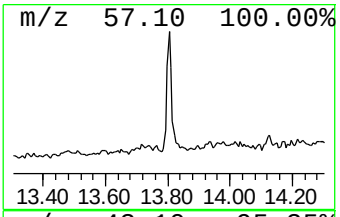
****

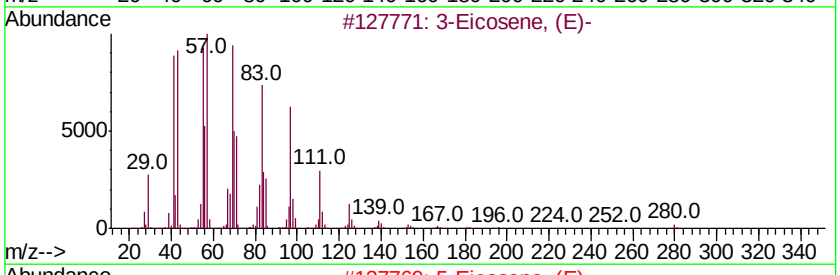
Peak Number 6 3-Eicosene, (E)- Concentration Rank 5

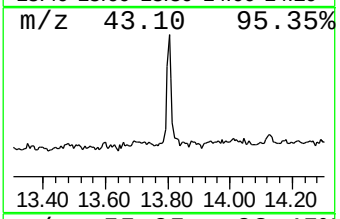
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	8.54 ng	407910	Chrysene-d12	13.95

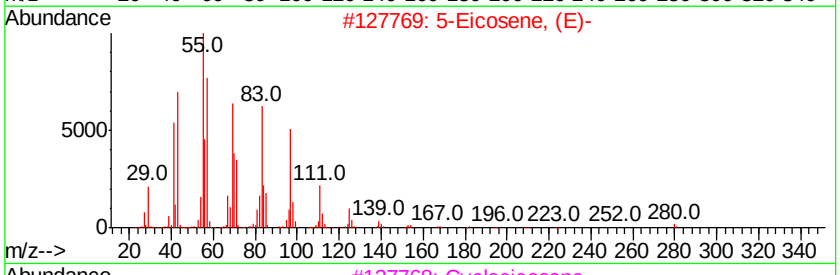
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	98
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
3	Cycloeicosane	280	C20H40	000296-56-0	96
4	1-Heneicosanol	312	C21H44O	015594-90-8	95
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	95

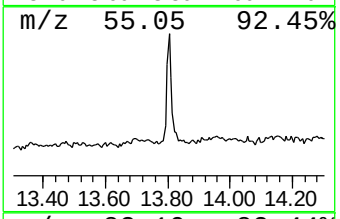


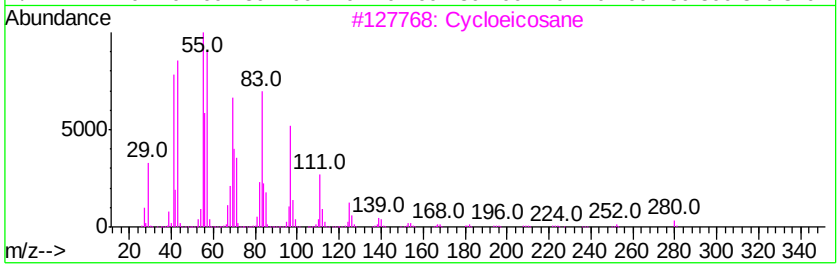


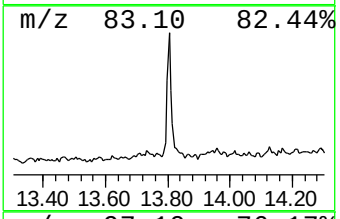


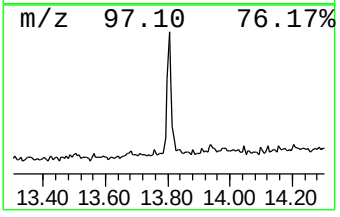












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121318\
Data File : BF111379.D
Acq On : 13 Dec 2018 19:36
Operator : JU/SJ
Sample : J6214-51
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.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
unknown6.56	6.56	73.6	ng	5157560	1	6.79	1401060	20.0
n-Hexadecanoic acid	11.85	15.6	ng	925332	4	11.31	1188970	20.0
Octadecanoic acid	12.63	11.2	ng	537268	5	13.95	955818	20.0
3-Eicosene, (E)-	13.80	8.5	ng	407910	5	13.95	955818	20.0