LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136389.D
Acq On : 04 Dec 2023 19:03
Operator : CG\JU
Sample : 05521-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2-COMP

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-BF112723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136389.D\data.ms

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	508	rBV	36740	48422	2.20%	0.264%
2	5.440	565	570	573	rBV	2127073	1923055	87.49%	10.482%
3	6.440	735	740	743	rBV	2100774	1873262	85.22%	10.211%
4	6.634	770	773	782	rBV	27103	39289	1.79%	0.214%
5	6.804	798	802	805	rBV	918632	749388	34.09%	4.085%
6	6.957	825	828	831	rBV	45125	35782	1.63%	0.195%
7	7.363	892	897	900	rBV	1455697	1217346	55.38%	6.636%
8	7.828	973	976	981	rVB	50182	43002	1.96%	0.234%
9	8.081	1015	1019	1022	rBV	1177231	939937	42.76%	5.123%
10	9.157	1198	1202	1205	rBV	2969283	2198062	100.00%	11.981%
11	9.275	1218	1222	1225	rBV	51662	45602	2.07%	0.249%
12	9.492	1256	1259	1262	rBV	89230	68220	3.10%	0.372%
13	9.539	1264	1267	1269	rBV	47857	35273	1.60%	0.192%
14	9.686	1288	1292	1298	rVB3	49462	51329	2.34%	0.280%
15	9.833	1310	1317	1321	rBV	1108045	1105274	50.28%	6.025%
16	9.881	1321	1325	1328	rVB	37505	40822	1.86%	0.223%
17	10.628	1448	1452	1455	rBV	1262596	1053575	47.93%	5.743%
18	11.280	1559	1563	1566	rBV3	42542	44917	2.04%	0.245%
19	11.328	1567	1571	1573	rVV	1025624	849654	38.65%	4.631%
20	11.351	1573	1575	1579	rVV	89458	82882	3.77%	0.452%
21	11.386	1579	1581	1586	rVB2	24287	36578	1.66%	0.199%
22	11.792	1646	1650	1654	rBV2	46213	66896	3.04%	0.365%
23	11.863	1658	1662	1671	rVB2	368590	378434	17.22%	2.063%
24	12.039	1689	1692	1702	rBV5	31000	41635	1.89%	0.227%
25	12.122	1702	1706	1709	rBV3	45057	51718	2.35%	0.282%
26	12.545	1773	1778	1781	rBV	220736	224372	10.21%	1.223%
27	12.592	1781	1786	1791	rVB9	33133	60407	2.75%	0.329%
28	12.651	1793	1796	1802	rBV3	81101	89895	4.09%	0.490%
29	12.774	1811	1817	1820	rBV	194405	194624	8.85%	1.061%
30	12.922	1838	1842	1846	rBV	2088795	1884483	85.73%	10.272%
31	12.992	1850	1854	1858	rBV4	19396	29535	1.34%	0.161%
32	13.169	1880	1884	1887	rBV3	31557	45530	2.07%	0.248%
33	13.504	1936	1941	1944	rBV2	30249	48497	2.21%	0.264%
34	13.857	1996	2001	2010	rBV4	81241	179049	8.15%	0.976%
35	13.980	2017	2022	2025	rBV	928180	922111	41.95%	5.026%
36	14.004	2025	2026	2029	rVB	103315	64223	2.92%	0.350%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136389.D
Acq On : 04 Dec 2023 19:03
Operator : CG\JU
Sample : 05521-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2-COMP

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-BF112723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.157	2050	2052	2056	rVB2	35266	29563	1.34%	0.161%
38	14.463	2101	2104	2107	rVB2	78931	68053	3.10%	0.371%
39	14.851	2167	2170	2173	rBV	38224	42148	1.92%	0.230%
40	14.921	2179	2182	2188	rVB	115443	123892	5.64%	0.675%
41	15.027	2197	2200	2203	rBV	77438	107202	4.88%	0.584%
42	15.121	2213	2216	2223	rVB2	151148	192637	8.76%	1.050%
43	15.398	2260	2263	2269	rVB	59556	72095	3.28%	0.393%
44	15.468	2270	2275	2278	rBV	424665	547994	24.93%	2.987%
45	15.974	2356	2361	2370	rVB	261085	399166	18.16%	2.176%

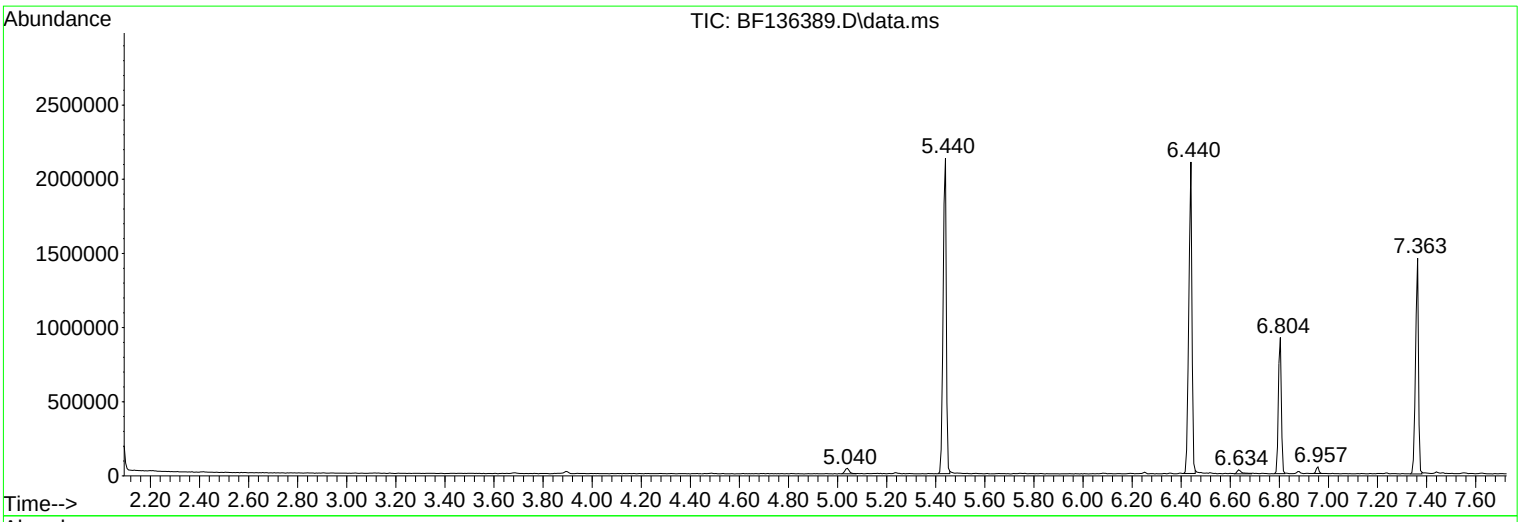
Sum of corrected areas: 18345830

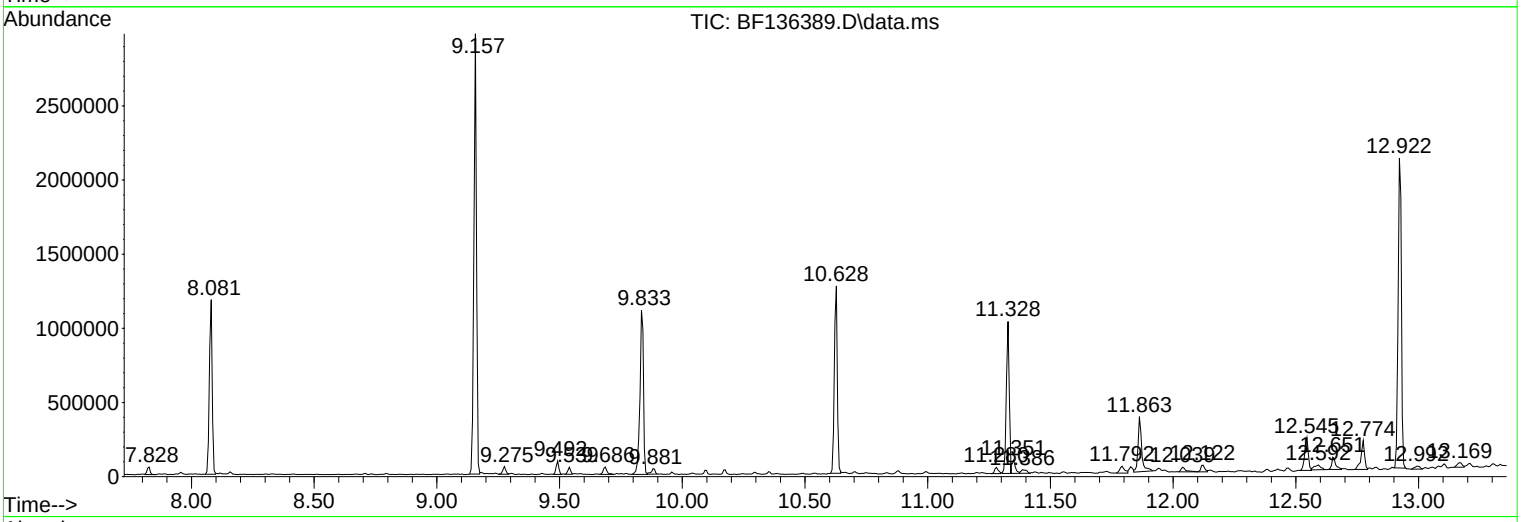
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136389.D
Acq On : 04 Dec 2023 19:03
Operator : CG\JU
Sample : 05521-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

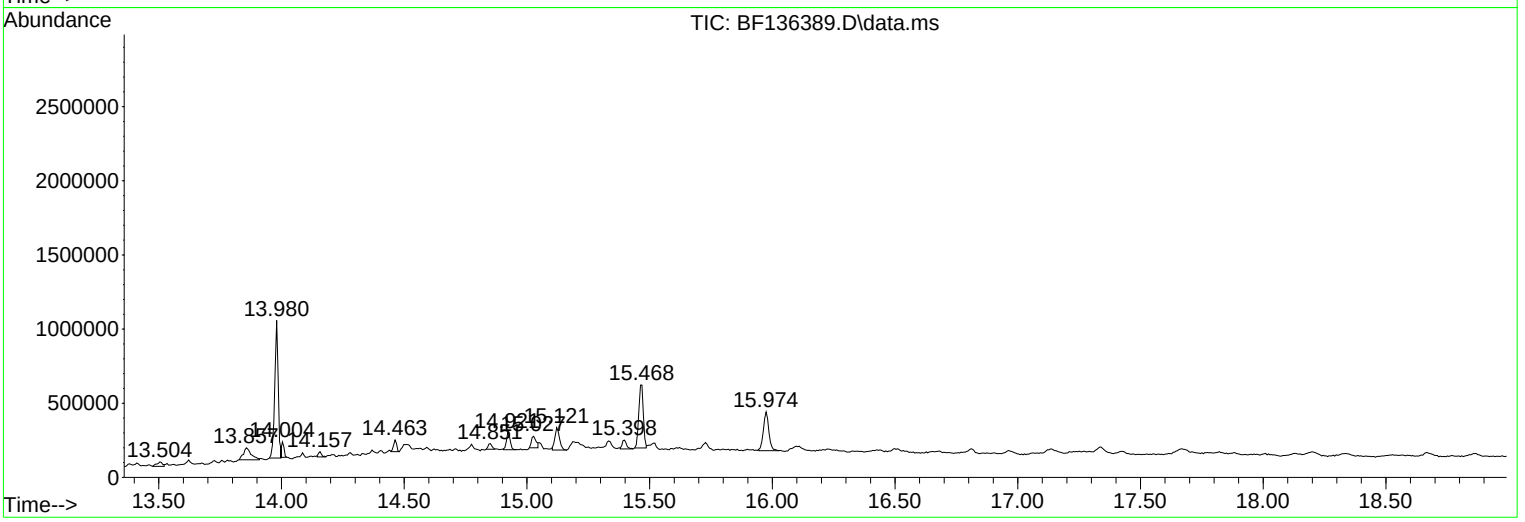
Instrument :
BNA_F
ClientSampleId :
SP-2-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136389.D
Acq On : 04 Dec 2023 19:03
Operator : CG\JU
Sample : 05521-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

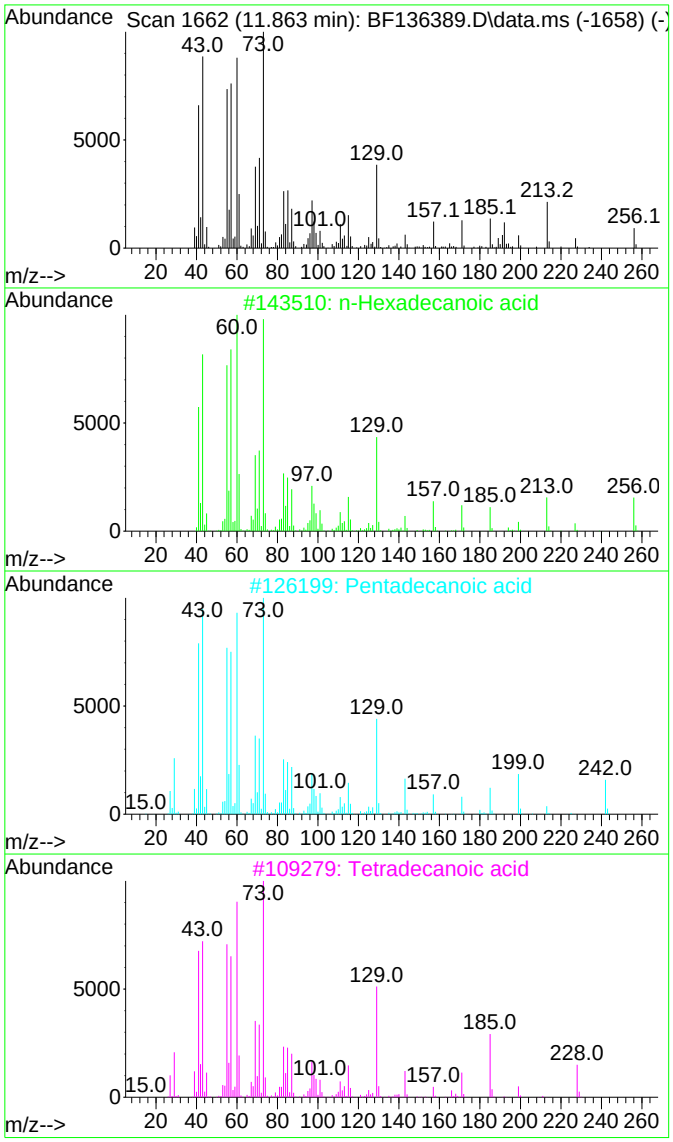
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

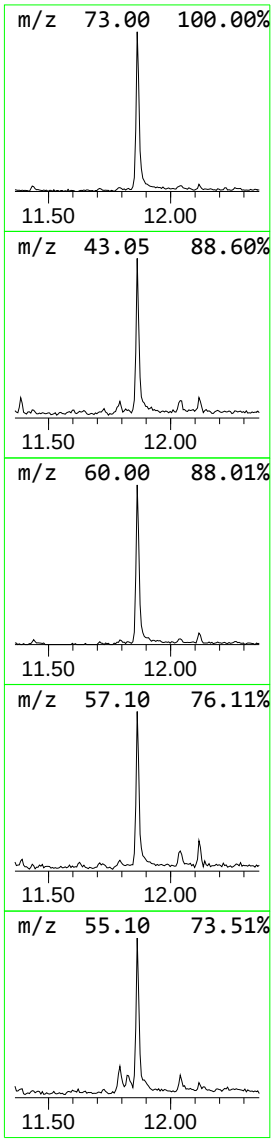
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	8.91 ng	378434	Phenanthrene-d10	11.328

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	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136389.D
Acq On : 04 Dec 2023 19:03
Operator : CG\JU
Sample : 05521-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

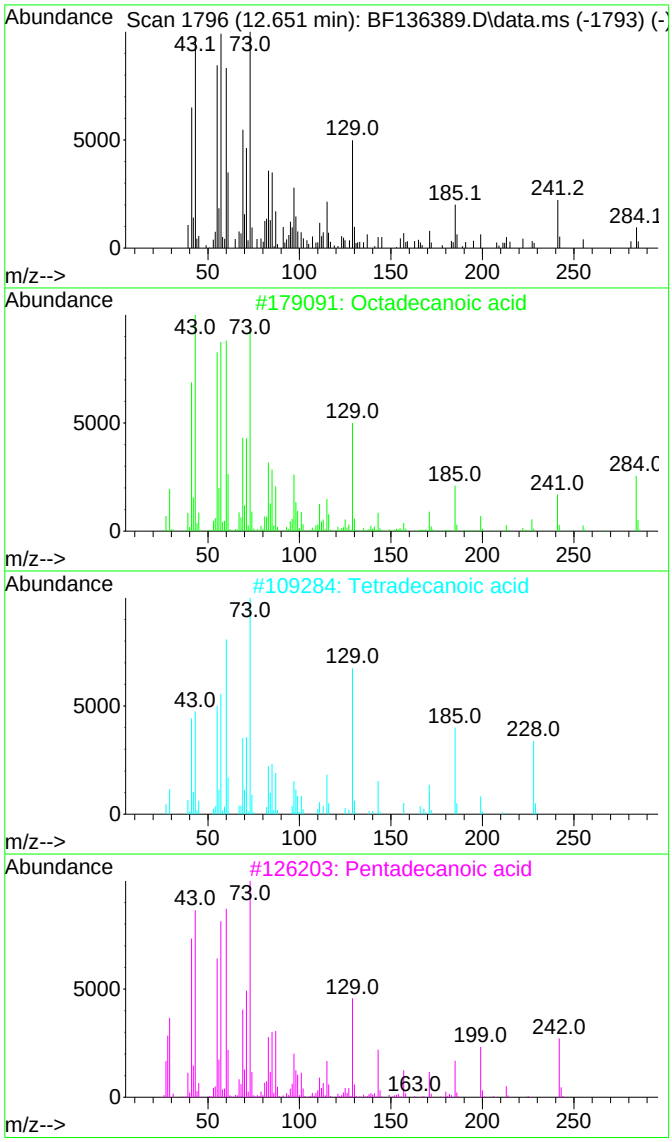
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

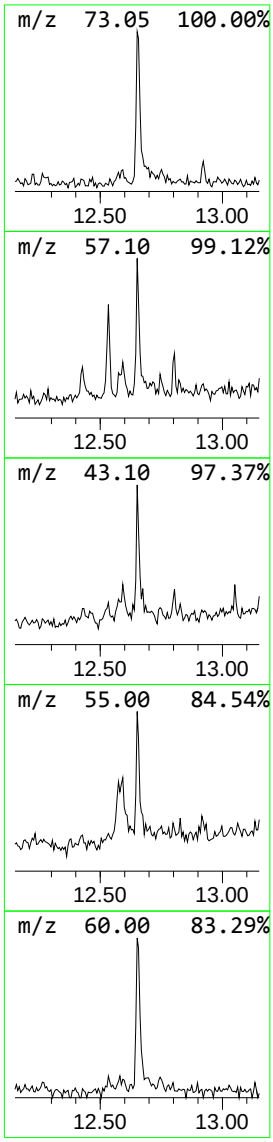
****

Peak Number 2 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	2.12 ng	89895	Phenanthrene-d10	11.328

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	n-Decanoic acid	172	C10H20O2	000334-48-5	46
5	Undecanoic acid	186	C11H22O2	000112-37-8	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136389.D
Acq On : 04 Dec 2023 19:03
Operator : CG\JU
Sample : 05521-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

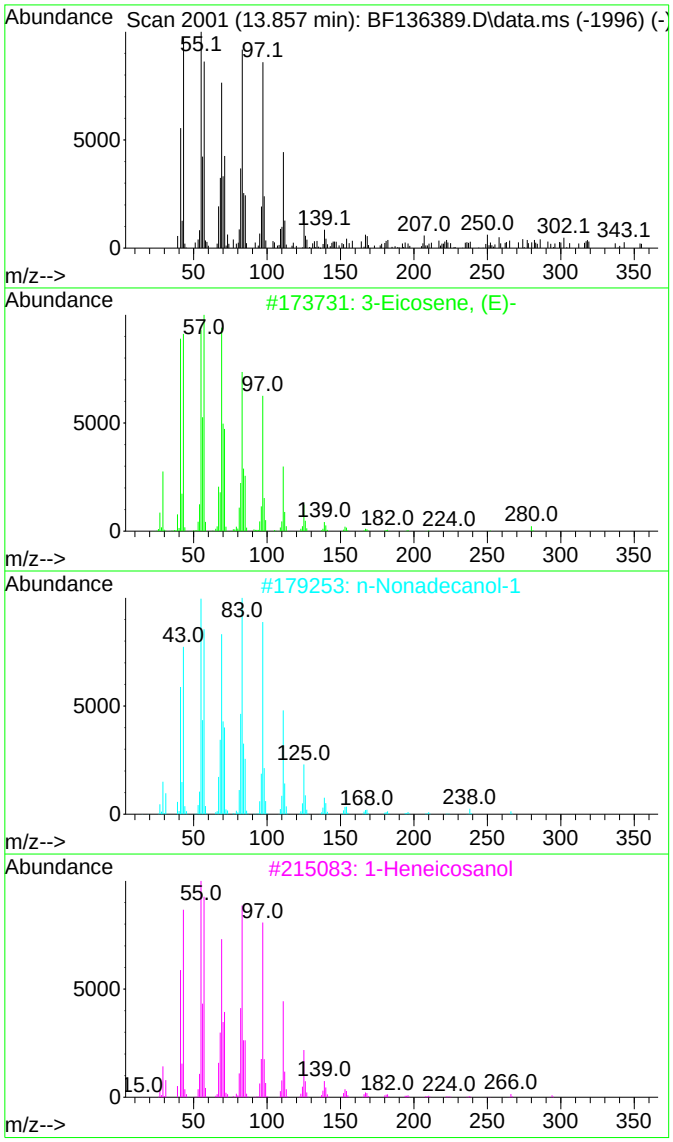
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

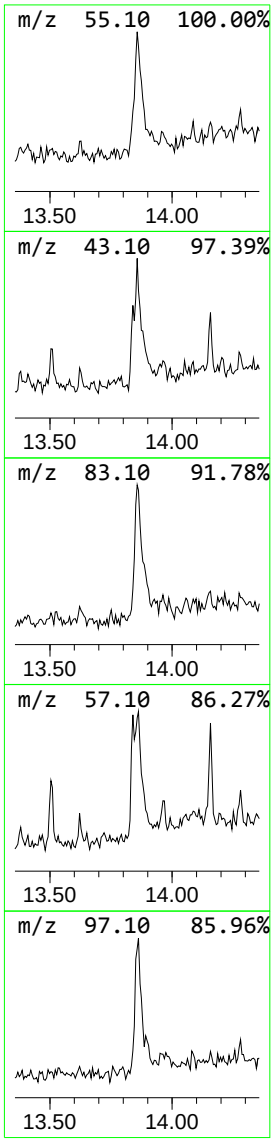
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	3.88 ng	179049	Chrysene-d12	13.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	96
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	1-Tricosene	322	C23H46	018835-32-0	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136389.D
Acq On : 04 Dec 2023 19:03
Operator : CG\JU
Sample : 05521-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

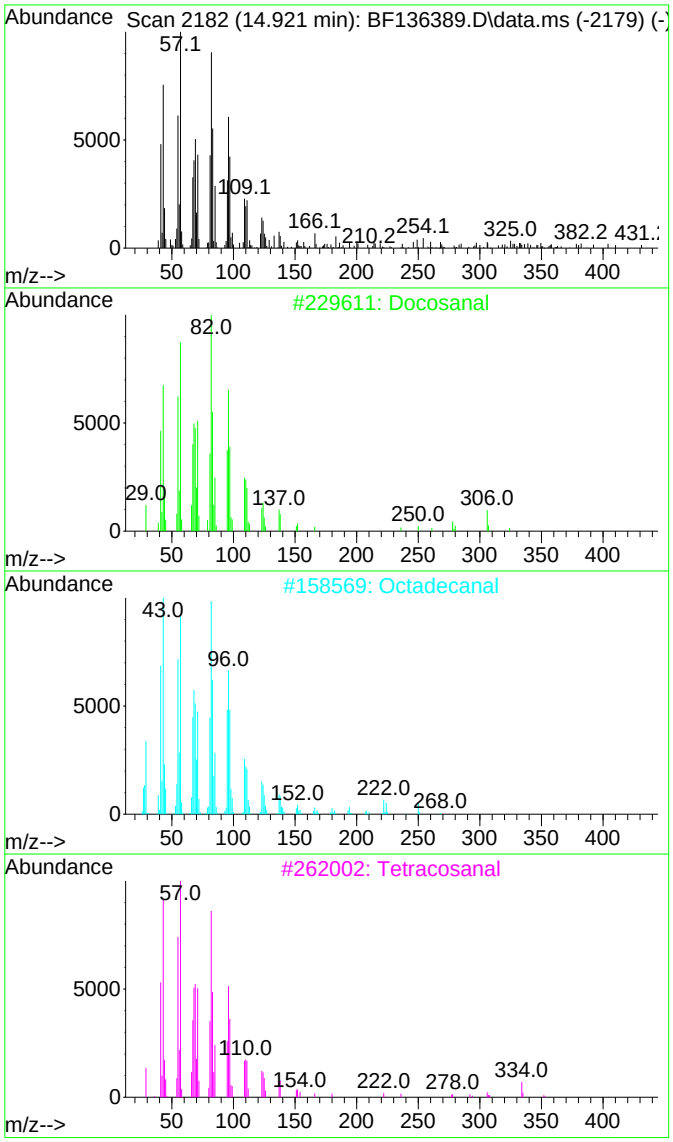
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

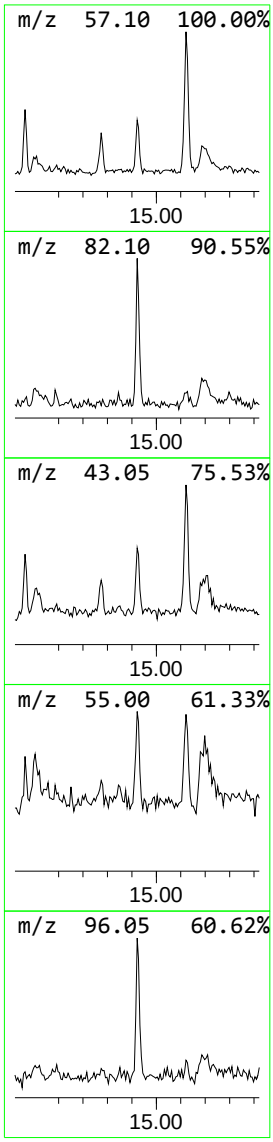
****

Peak Number 4 Docosanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.921	4.52 ng	123892	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanal	324	C22H44O	057402-36-5	94
2	Octadecanal	268	C18H36O	000638-66-4	91
3	Tetracosanal	352	C24H48O	057866-08-7	91
4	Nonacosanal	422	C29H58O	072934-04-4	91
5	Eicosanal-	296	C20H40O	002400-66-0	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136389.D
Acq On : 04 Dec 2023 19:03
Operator : CG\JU
Sample : 05521-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2-COMP

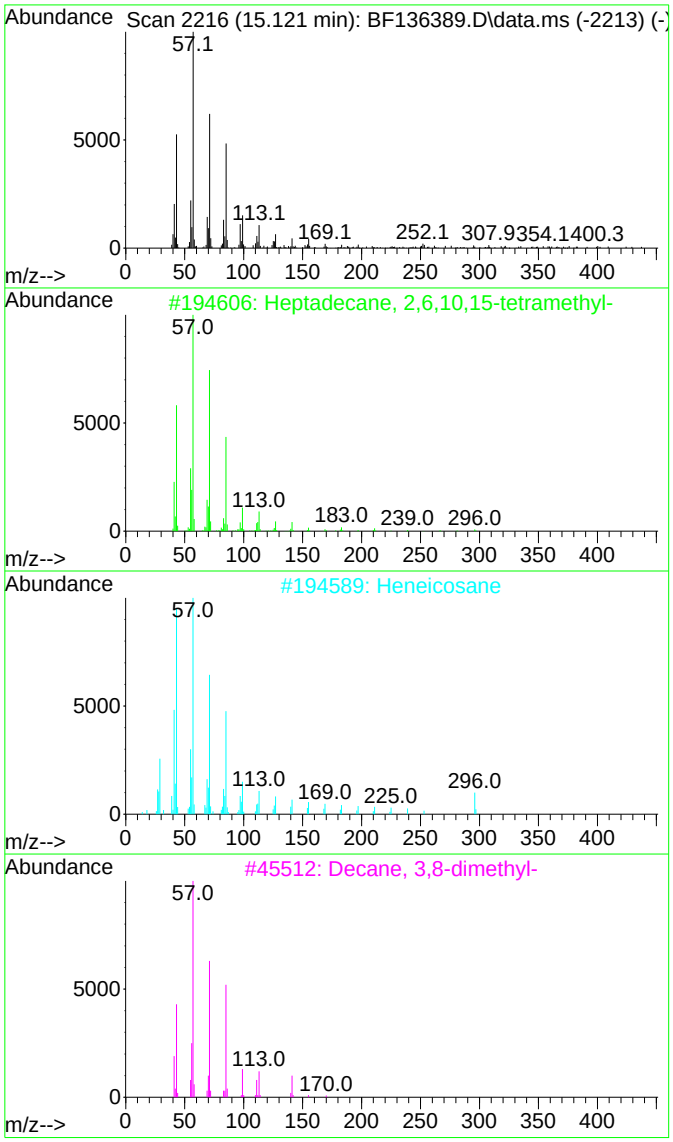
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

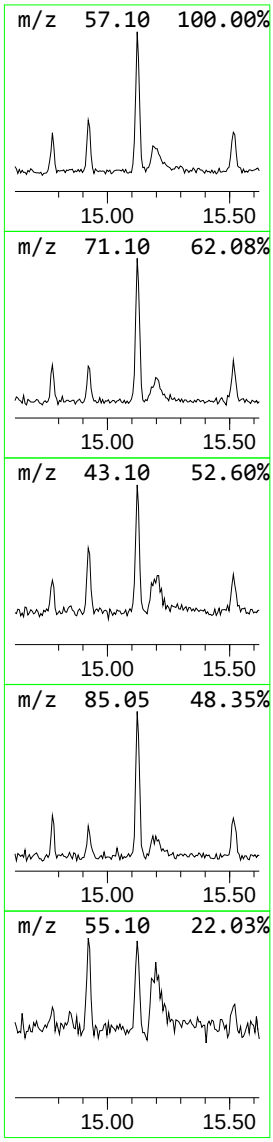
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Heptadecane, 2,6,10,15-tetr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.121	7.03 ng	192637	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5	Octacosane	394	C28H58	000630-02-4	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136389.D
Acq On : 04 Dec 2023 19:03
Operator : CG\JU
Sample : 05521-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

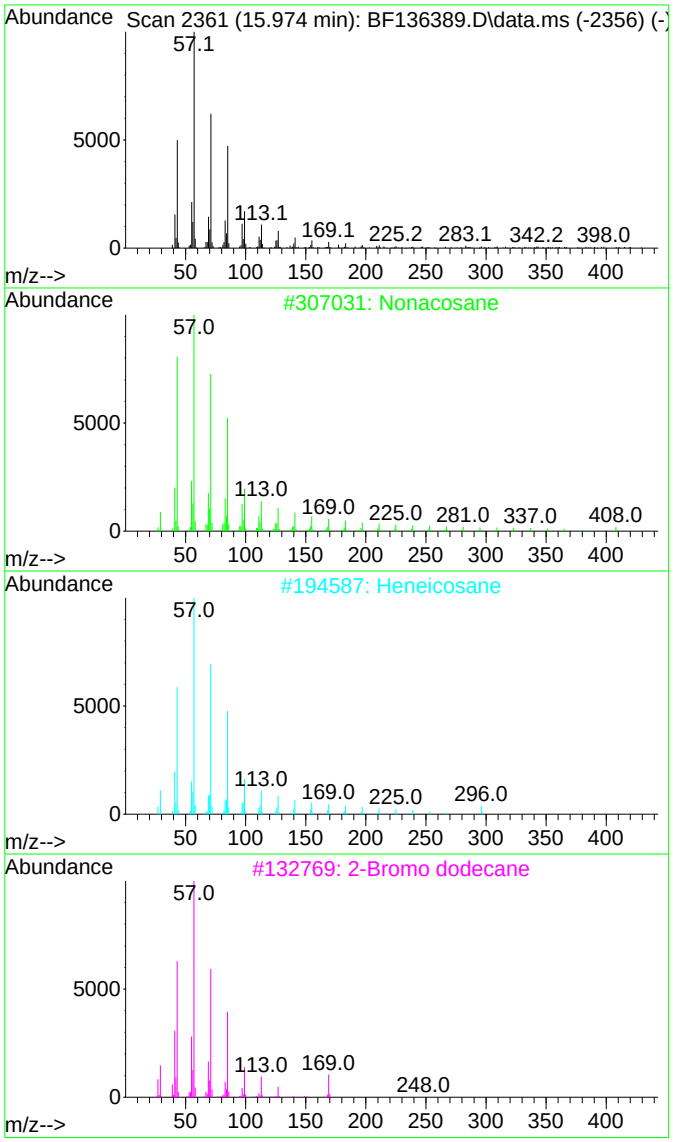
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

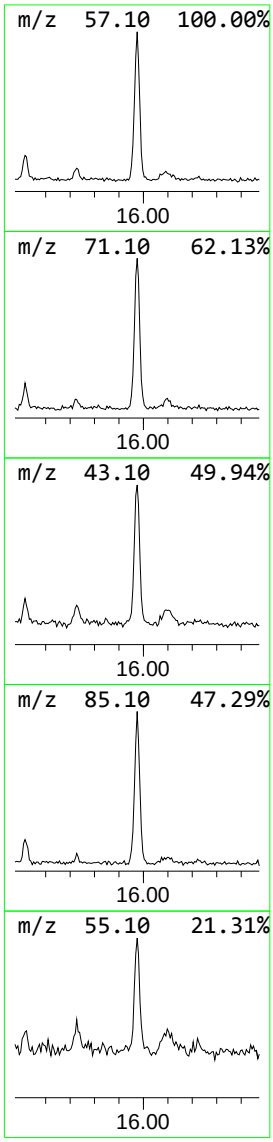
****

Peak Number 6 Nonacosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.974	14.57 ng	399166	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacosane	408	C29H60	000630-03-5	94
2	Heneicosane	296	C21H44	000629-94-7	93
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
5	Hexacosane	366	C26H54	000630-01-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120423\
Data File : BF136389.D
Acq On : 04 Dec 2023 19:03
Operator : CG\JU
Sample : 05521-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic ...	11.863	8.9	ng	378434	4	11.328	849654	20.0
Octadecanoic acid	12.651	2.1	ng	89895	4	11.328	849654	20.0
3-Eicosene, (E)-	13.857	3.9	ng	179049	5	13.980	922111	20.0
Docosanal	14.921	4.5	ng	123892	6	15.468	547994	20.0
Heptadecane, 2,...	15.121	7.0	ng	192637	6	15.468	547994	20.0
Nonacosane	15.974	14.6	ng	399166	6	15.468	547994	20.0