LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080522\
Data File : BM036138.D
Acq On : 06 Aug 2022 02:44
Operator : CG/JU
Sample : N3960-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-164

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_M\Methods\8270-BM080122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036138.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.957	311	318	323	rBV	90987	128167	1.41%	0.205%
2	5.446	394	401	413	rBV	3231555	4582774	50.47%	7.315%
3	7.069	669	677	687	rBV	3079353	4737903	52.18%	7.562%
4	7.857	803	811	819	rBV	1006598	1562923	17.21%	2.495%
5	9.028	1002	1010	1024	rBV	1934642	3170390	34.92%	5.060%
6	10.657	1280	1287	1294	rBV	1299599	2189755	24.12%	3.495%
7	12.327	1563	1571	1581	rBV3	30281	91293	1.01%	0.146%
8	13.121	1698	1706	1718	rBV	5004427	7177425	79.05%	11.456%
9	14.151	1874	1881	1887	rBV3	79998	152829	1.68%	0.244%
10	14.221	1887	1893	1901	rVB	139928	220534	2.43%	0.352%
11	14.498	1933	1940	1948	rBV	1855571	2753411	30.33%	4.395%
12	15.986	2185	2193	2199	rBV	3686051	5484938	60.41%	8.755%
13	16.204	2226	2230	2240	rBV6	42275	110811	1.22%	0.177%
14	17.145	2385	2390	2397	rBV5	53773	116831	1.29%	0.186%
15	17.239	2398	2406	2410	rVV	2168066	2985000	32.88%	4.764%
16	17.280	2410	2413	2417	rVB	234637	290039	3.19%	0.463%
17	17.368	2424	2428	2434	rVB	97821	135493	1.49%	0.216%
18	17.627	2464	2472	2481	rBV3	128793	272184	3.00%	0.434%
19	17.909	2516	2520	2525	rVB	195361	237144	2.61%	0.379%
20	18.139	2552	2559	2567	rBV3	493295	844135	9.30%	1.347%
21	18.209	2567	2571	2574	rBV	200985	225836	2.49%	0.360%
22	18.304	2583	2587	2592	rBV2	89045	169873	1.87%	0.271%
23	18.427	2605	2608	2614	rBV3	60462	104920	1.16%	0.167%
24	18.998	2701	2705	2708	rBV	188640	255013	2.81%	0.407%
25	19.027	2708	2710	2714	rVV	111898	173904	1.92%	0.278%
26	19.086	2716	2720	2724	rVB2	483028	577214	6.36%	0.921%
27	19.215	2739	2742	2748	rVB	172945	199342	2.20%	0.318%
28	19.292	2751	2755	2762	rBV	428475	744757	8.20%	1.189%
29	19.415	2774	2776	2779	rBV2	88760	95245	1.05%	0.152%
30	19.656	2813	2817	2825	rVB	582797	870112	9.58%	1.389%
31	19.862	2847	2852	2857	rBV	7745712	9079615	100.00%	14.492%
32	20.145	2898	2900	2903	rBV2	100651	97471	1.07%	0.156%
33	20.450	2949	2952	2956	rBV	142099	179746	1.98%	0.287%
34	21.127	3064	3067	3074	rVB3	1068844	1361427	14.99%	2.173%
35	21.415	3111	3116	3120	rBV	2725629	3632119	40.00%	5.797%
36	23.050	3390	3394	3399	rBV2	888377	1501556	16.54%	2.397%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080522\
Data File : BM036138.D
Acq On : 06 Aug 2022 02:44
Operator : CG/JU
Sample : N3960-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-164

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_M\Methods\8270-BM080122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.103	3401	3403	3416	rVB2	698543	1131532	12.46%	1.806%
38	23.774	3512	3517	3524	rVB2	1573091	3021436	33.28%	4.823%
39	24.374	3615	3619	3628	rVB	955300	1985798	21.87%	3.170%

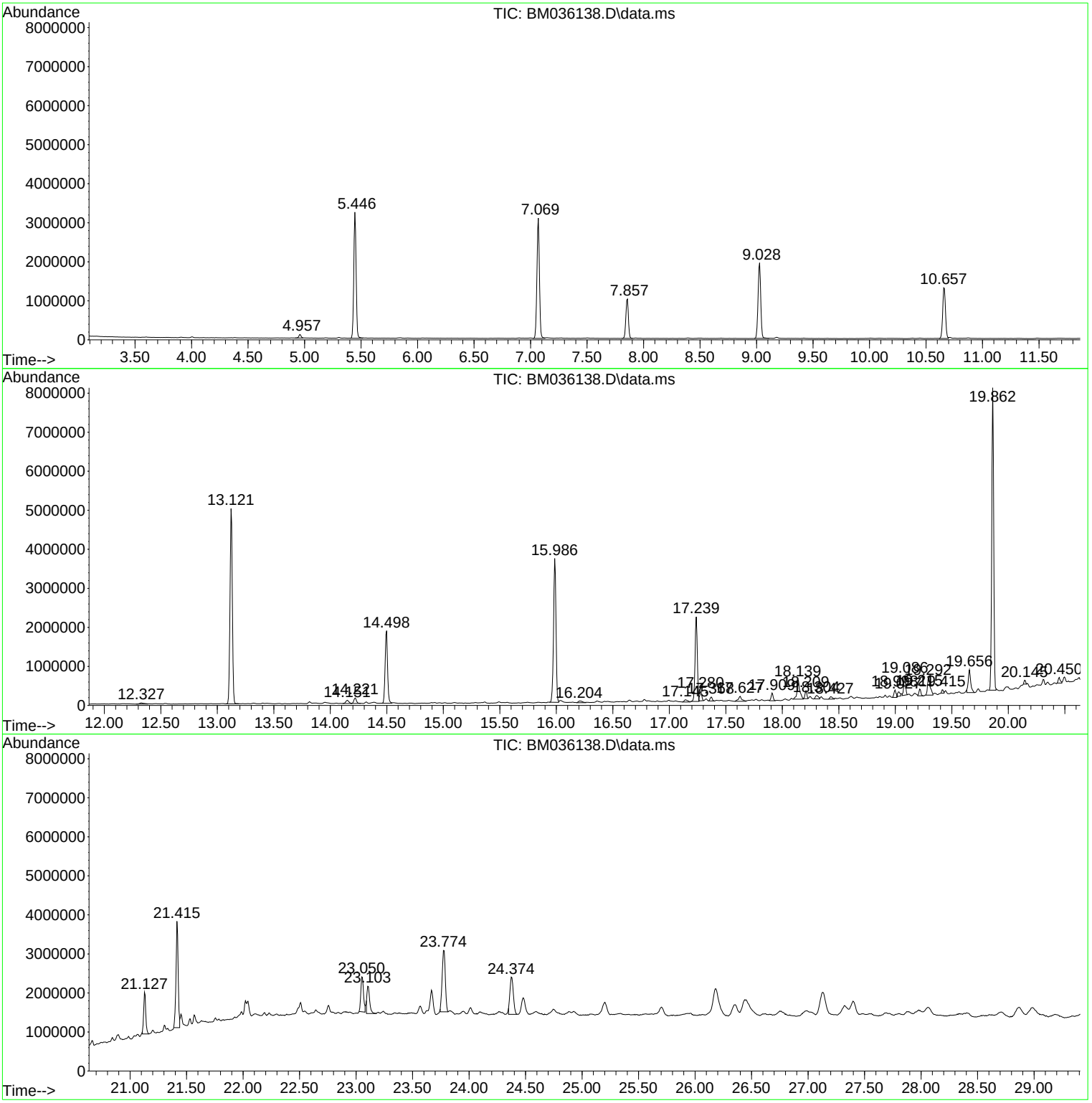
Sum of corrected areas: 62650895

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080522\
Data File : BM036138.D
Acq On : 06 Aug 2022 02:44
Operator : CG/JU
Sample : N3960-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-164

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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_M\Data\BM080522\
Data File : BM036138.D
Acq On : 06 Aug 2022 02:44
Operator : CG/JU
Sample : N3960-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-164

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

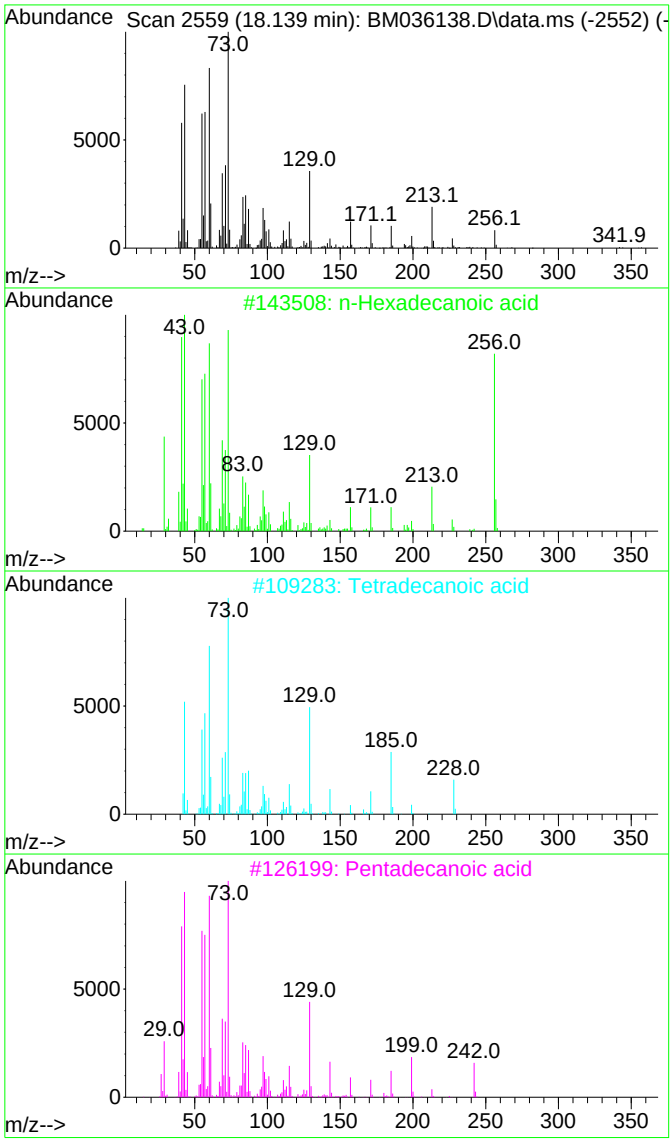
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

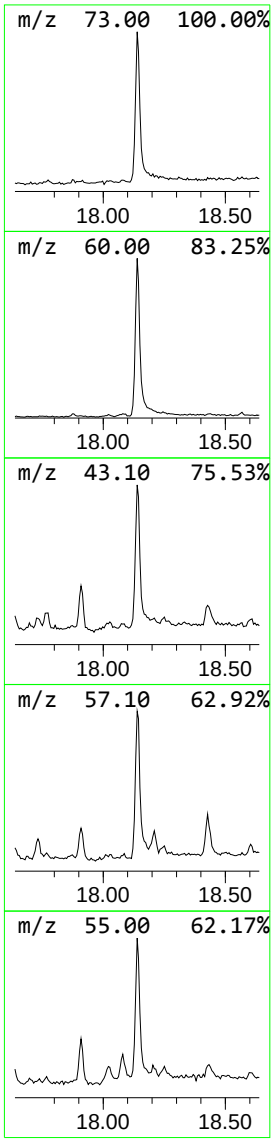
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.139	5.66 ng	844135	Phenanthrene-d10	17.239

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	Octadecanoic acid	284	C18H36O2	000057-11-4	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080522\
Data File : BM036138.D
Acq On : 06 Aug 2022 02:44
Operator : CG/JU
Sample : N3960-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-164

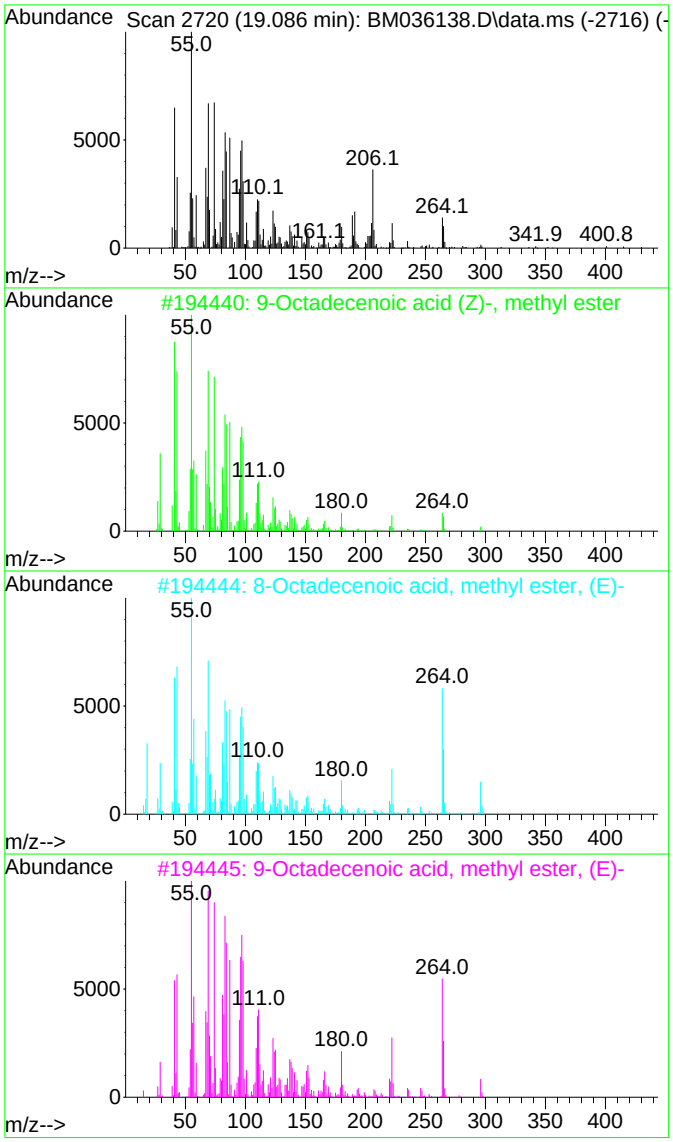
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

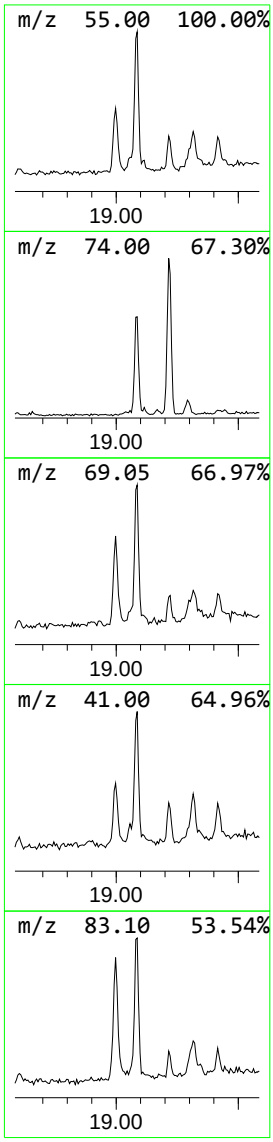
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 9-Octadecenoic acid (Z)-, m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.086	3.87 ng	577214	Phenanthrene-d10	17.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	8-Octadecenoic acid, methyl este...	296	C19H36O2	026528-50-7	99
3	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
4	7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	99
5	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080522\
Data File : BM036138.D
Acq On : 06 Aug 2022 02:44
Operator : CG/JU
Sample : N3960-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-164

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

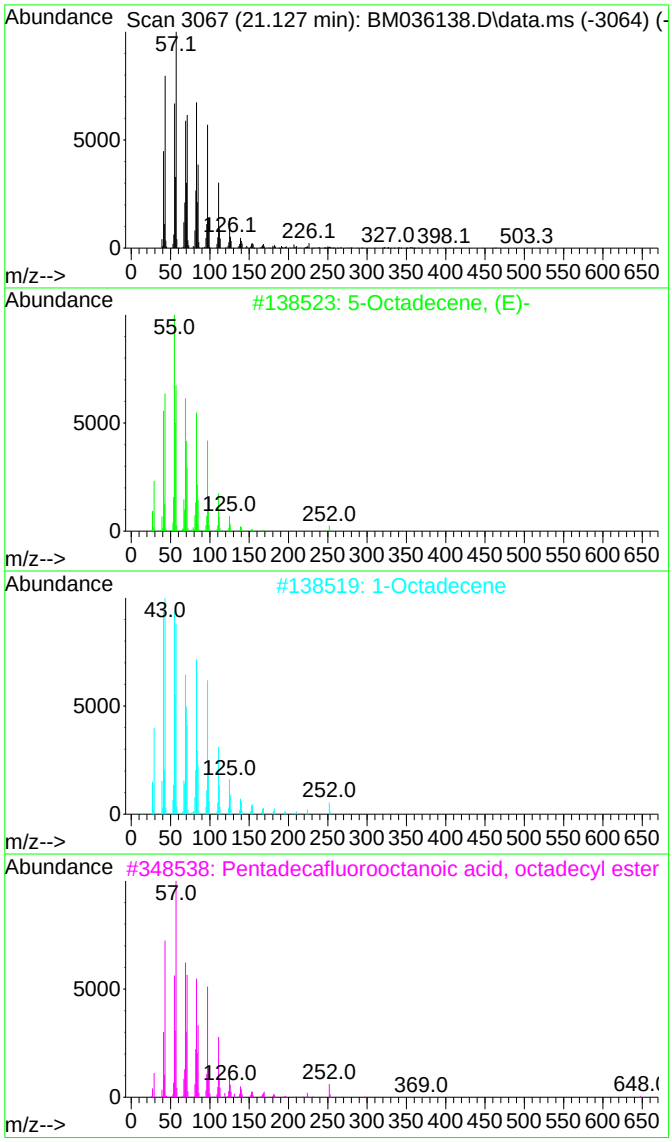
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

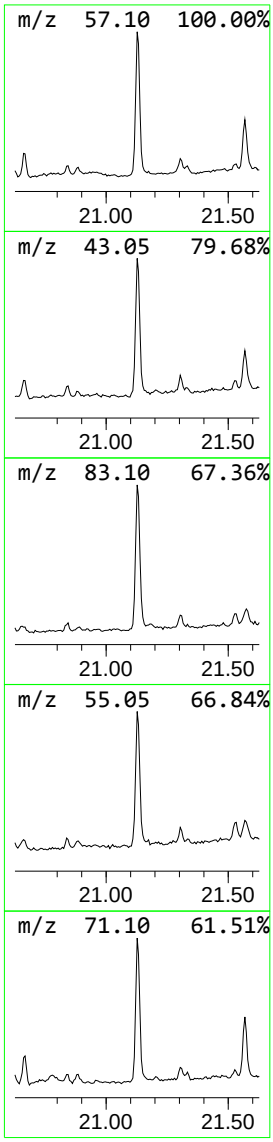
****

Peak Number 3 5-Octadecene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	7.50 ng	1361430	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
2	1-Octadecene	252	C18H36	000112-88-9	94
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080522\
Data File : BM036138.D
Acq On : 06 Aug 2022 02:44
Operator : CG/JU
Sample : N3960-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-164

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

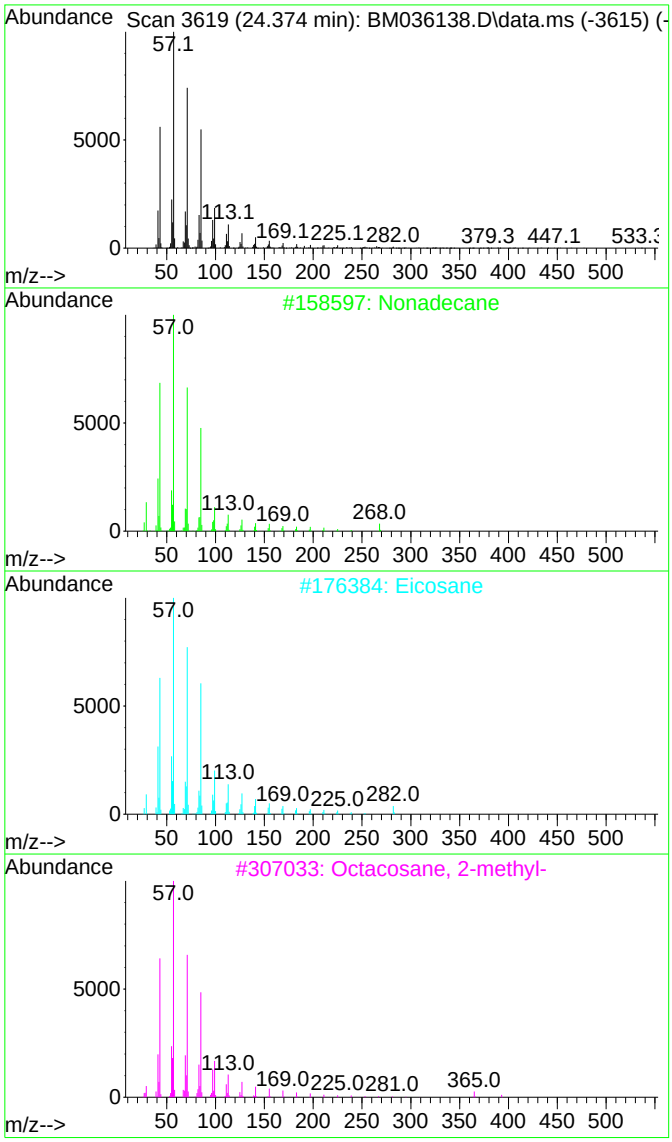
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

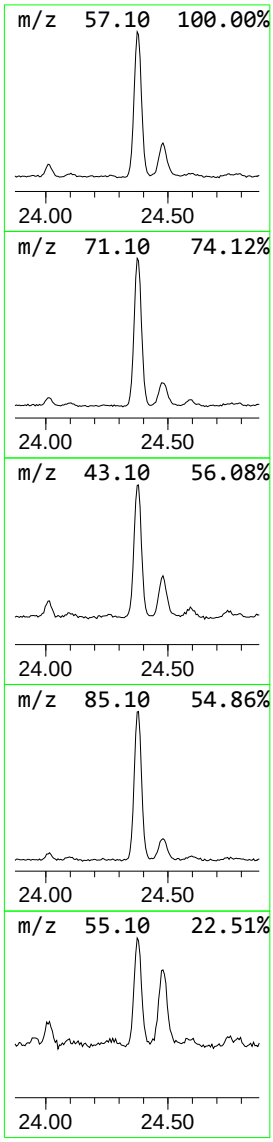
****

Peak Number 4 Nonadecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.374	13.14 ng	1985800	Perylene-d12	23.780

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Eicosane	282	C20H42	000112-95-8	94
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Heneicosane	296	C21H44	000629-94-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080522\
Data File : BM036138.D
Acq On : 06 Aug 2022 02:44
Operator : CG/JU
Sample : N3960-17
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-164

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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 ...	18.139	5.7	ng	844135	4	17.239	2985000	20.0
9-Octadecenoic ...	19.086	3.9	ng	577214	4	17.239	2985000	20.0
5-Octadecene, (E)-	21.127	7.5	ng	1361430	5	21.415	3632120	20.0
Nonadecane	24.374	13.1	ng	1985800	6	23.780	3021440	20.0