LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044814.D
Acq On : 29 Mar 2024 13:11
Operator : MA/JU
Sample : P1879-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : EB-01(2-4)

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-BM032824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM044814.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.499	66	70	78	rBV	53324	84163	2.13%	0.309%
2	5.275	366	372	381	rBV	1708577	2464701	62.48%	9.062%
3	6.846	630	639	651	rBV	1634775	2580595	65.41%	9.489%
4	7.663	770	778	785	rBV	394941	623472	15.80%	2.292%
5	8.828	968	976	988	rBV	954461	1626555	41.23%	5.981%
6	10.445	1239	1251	1257	rBV	467903	819547	20.77%	3.013%
7	11.204	1373	1380	1387	rBV2	19404	41101	1.04%	0.151%
8	12.928	1666	1673	1684	rBV	2011543	2947687	74.72%	10.838%
9	14.310	1900	1908	1915	rBV	641223	963006	24.41%	3.541%
10	15.810	2154	2163	2182	rBV	1642268	2424925	61.47%	8.916%
11	17.069	2370	2377	2381	rBV	777596	1118173	28.34%	4.111%
12	17.110	2381	2384	2389	rVB	187802	249884	6.33%	0.919%
13	17.204	2395	2400	2405	rVB	35368	50409	1.28%	0.185%
14	17.468	2441	2445	2454	rBV3	20212	43360	1.10%	0.159%
15	17.945	2520	2526	2528	rBV	58965	81778	2.07%	0.301%
16	17.980	2528	2532	2544	rVB2	571323	879413	22.29%	3.234%
17	18.139	2554	2559	2563	rBV2	53716	101029	2.56%	0.371%
18	18.180	2563	2566	2572	rVB	37963	51149	1.30%	0.188%
19	18.457	2608	2613	2617	rBV	28187	42762	1.08%	0.157%
20	18.845	2674	2679	2688	rBV2	297821	530410	13.44%	1.950%
21	19.015	2703	2708	2714	rBV6	34542	61838	1.57%	0.227%
22	19.133	2722	2728	2738	rBV	266029	448105	11.36%	1.648%
23	19.268	2747	2751	2761	rBV2	274264	402038	10.19%	1.478%
24	19.498	2782	2790	2799	rVB	300838	469139	11.89%	1.725%
25	19.715	2821	2827	2832	rBV	3127523	3945058	100.00%	14.506%
26	19.821	2842	2845	2853	rBV6	30184	67522	1.71%	0.248%
27	19.968	2865	2870	2872	rBV5	30096	56178	1.42%	0.207%
28	19.998	2872	2875	2879	rVB2	47600	68889	1.75%	0.253%
29	20.157	2898	2902	2907	rVB4	47763	64532	1.64%	0.237%
30	20.292	2922	2925	2930	rBV	30195	43739	1.11%	0.161%
31	20.345	2931	2934	2939	rVB2	29943	41100	1.04%	0.151%
32	20.751	3000	3003	3009	rVB	33148	50381	1.28%	0.185%
33	20.998	3041	3045	3051	rBV3	252424	342015	8.67%	1.258%
34	21.268	3084	3091	3095	rBV2	1099326	1605013	40.68%	5.901%
35	21.304	3095	3097	3105	rVB	172312	210500	5.34%	0.774%
36	22.333	3269	3272	3280	rVB2	181127	250214	6.34%	0.920%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044814.D
Acq On : 29 Mar 2024 13:11
Operator : MA/JU
Sample : P1879-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-01(2-4)

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-BM032824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.498	3465	3470	3478	rBV	746566	1346361	34.13%	4.950%

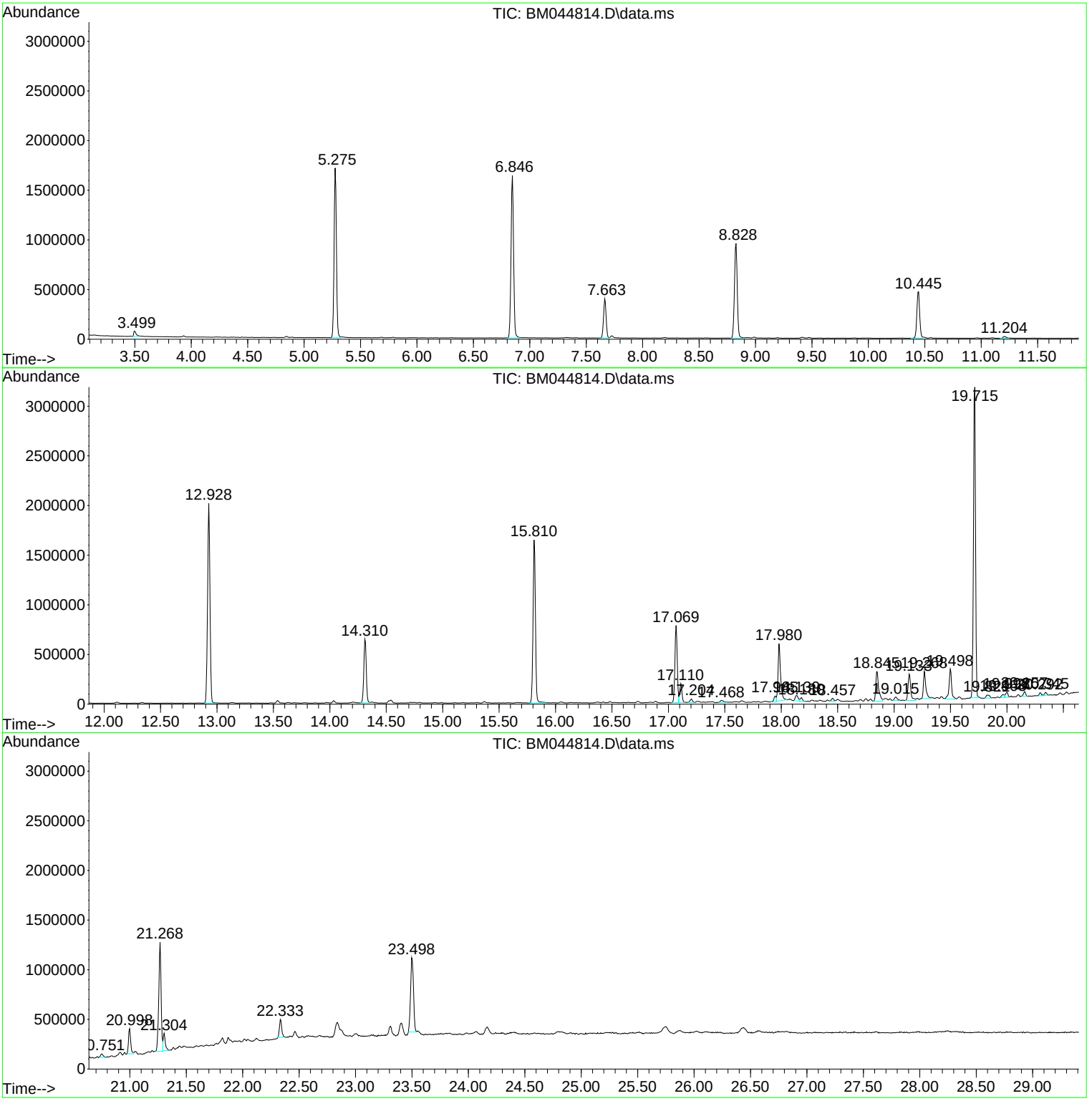
Sum of corrected areas: 27196741

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044814.D
Acq On : 29 Mar 2024 13:11
Operator : MA/JU
Sample : P1879-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-01(2-4)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.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\BM032924\
Data File : BM044814.D
Acq On : 29 Mar 2024 13:11
Operator : MA/JU
Sample : P1879-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-01(2-4)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

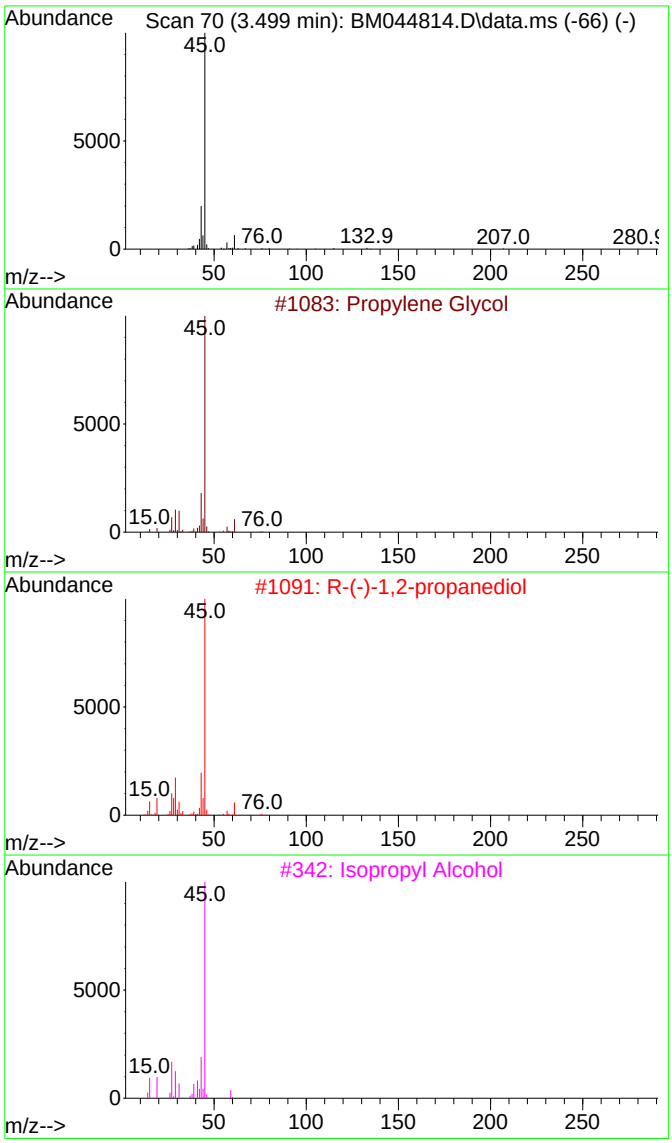
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

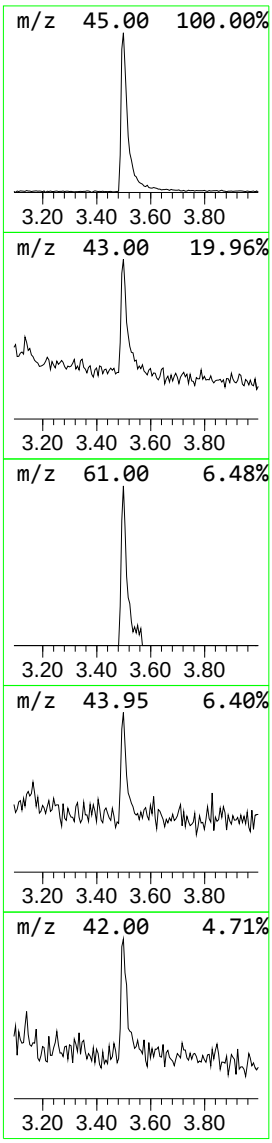
****

Peak Number 1 Propylene Glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.499	2.70 ng	84163	1,4-Dichlorobenzene-d4	7.663

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	86
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5	2-Hexanol, 3-methyl-	116	C7H16O	002313-65-7	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044814.D
Acq On : 29 Mar 2024 13:11
Operator : MA/JU
Sample : P1879-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-01(2-4)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

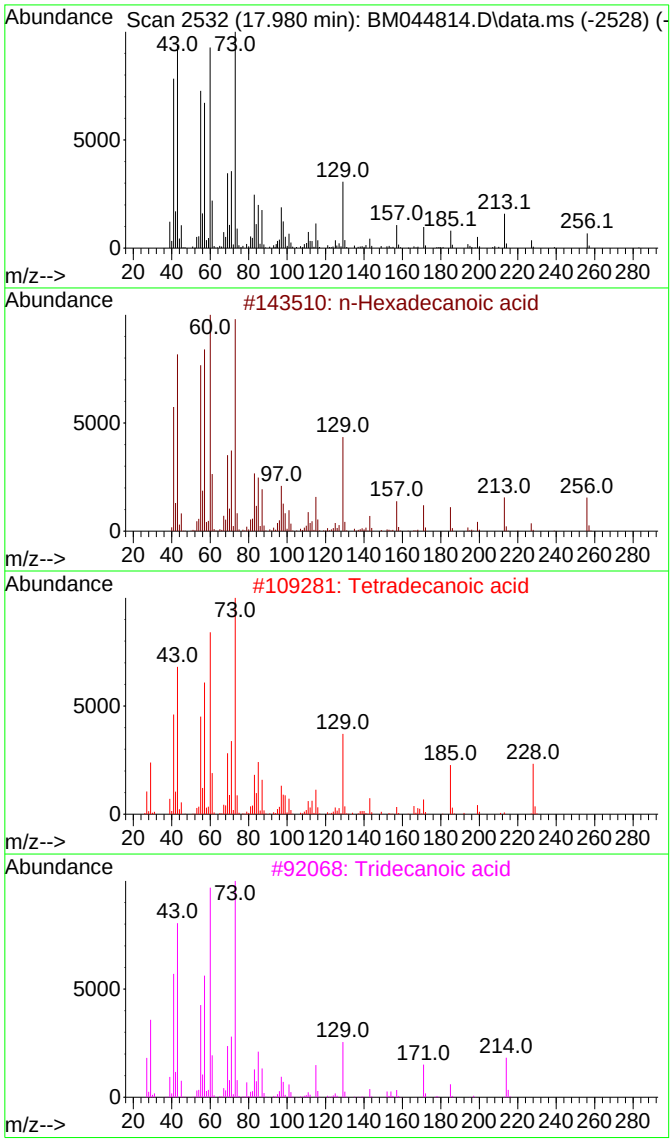
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

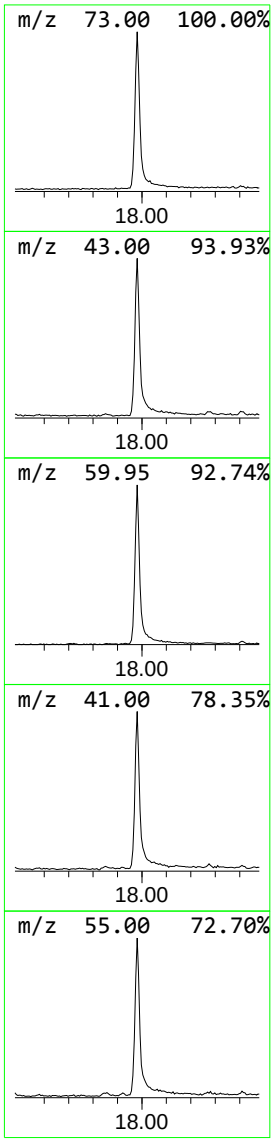
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.980	15.73 ng	879413	Phenanthrene-d10	17.069

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	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044814.D
Acq On : 29 Mar 2024 13:11
Operator : MA/JU
Sample : P1879-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-01(2-4)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

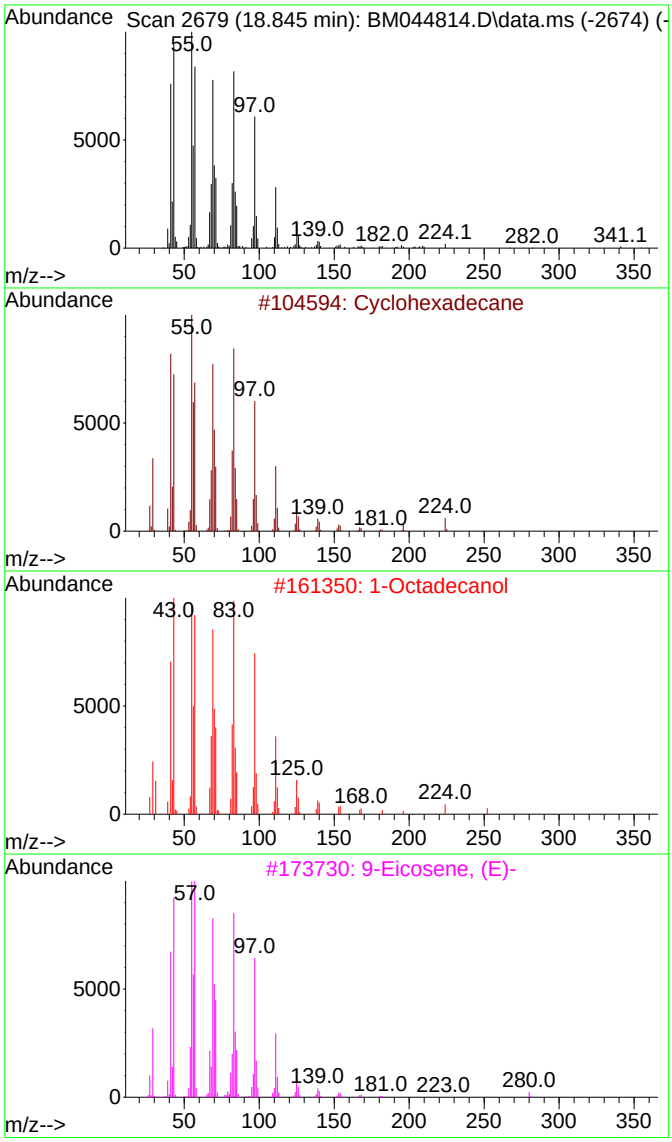
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

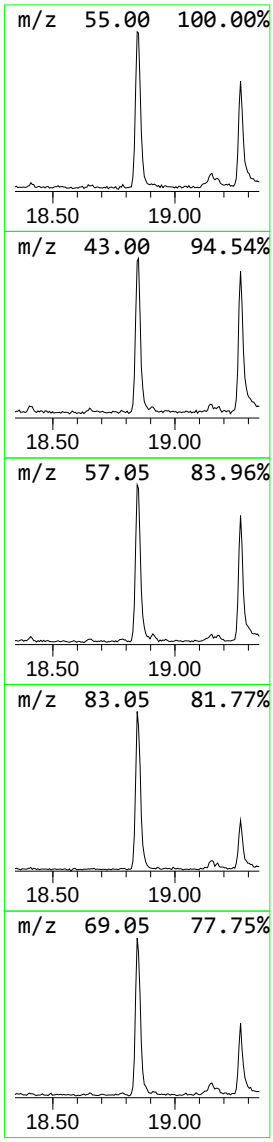
****

Peak Number 3 Cyclohexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.845	9.49 ng	530410	Phenanthrene-d10	17.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	94
2	1-Octadecanol	270	C18H38O	000112-92-5	94
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	94
4	1-Hexadecanol	242	C16H34O	036653-82-4	94
5	E-15-Heptadecenal	252	C17H32O	1000130-97-9	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044814.D
Acq On : 29 Mar 2024 13:11
Operator : MA/JU
Sample : P1879-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-01(2-4)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

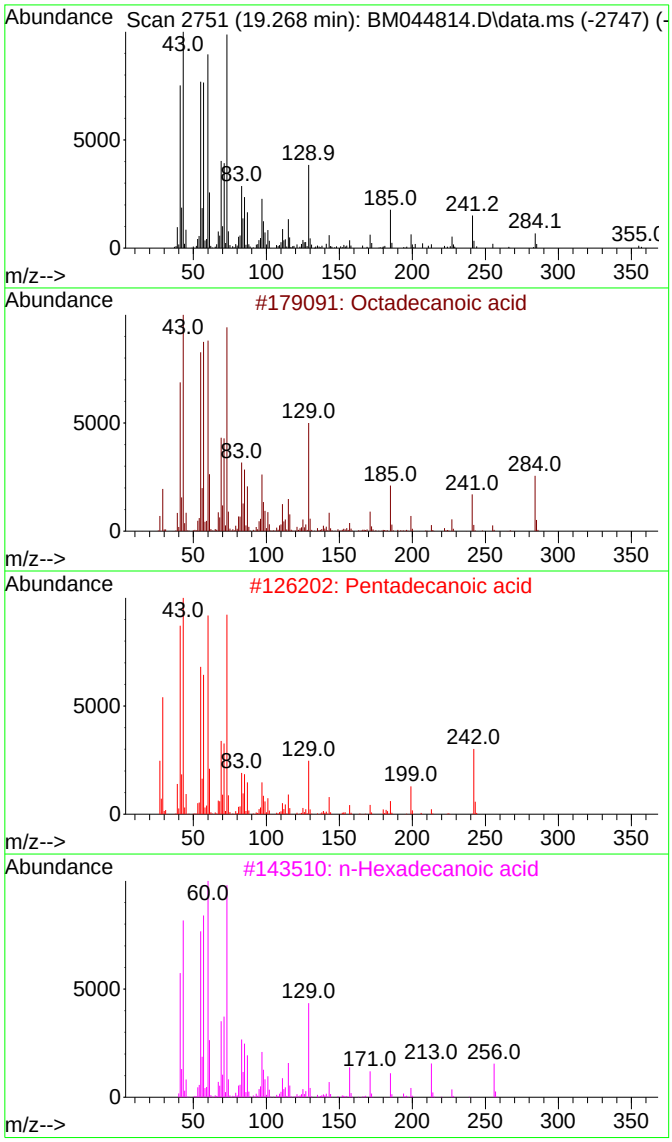
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

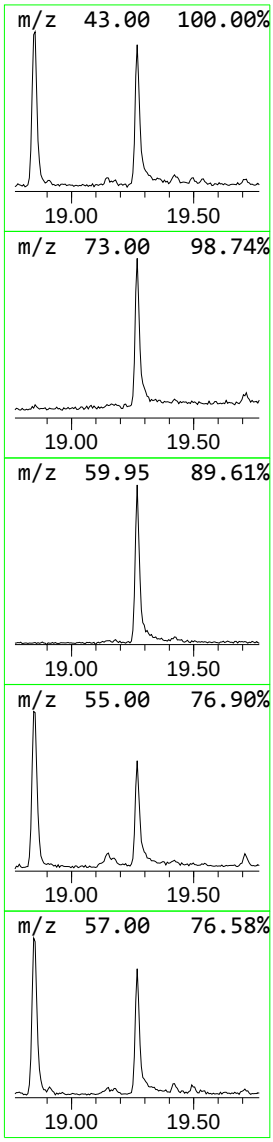
****

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.268	5.01 ng	402038	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044814.D
Acq On : 29 Mar 2024 13:11
Operator : MA/JU
Sample : P1879-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-01(2-4)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

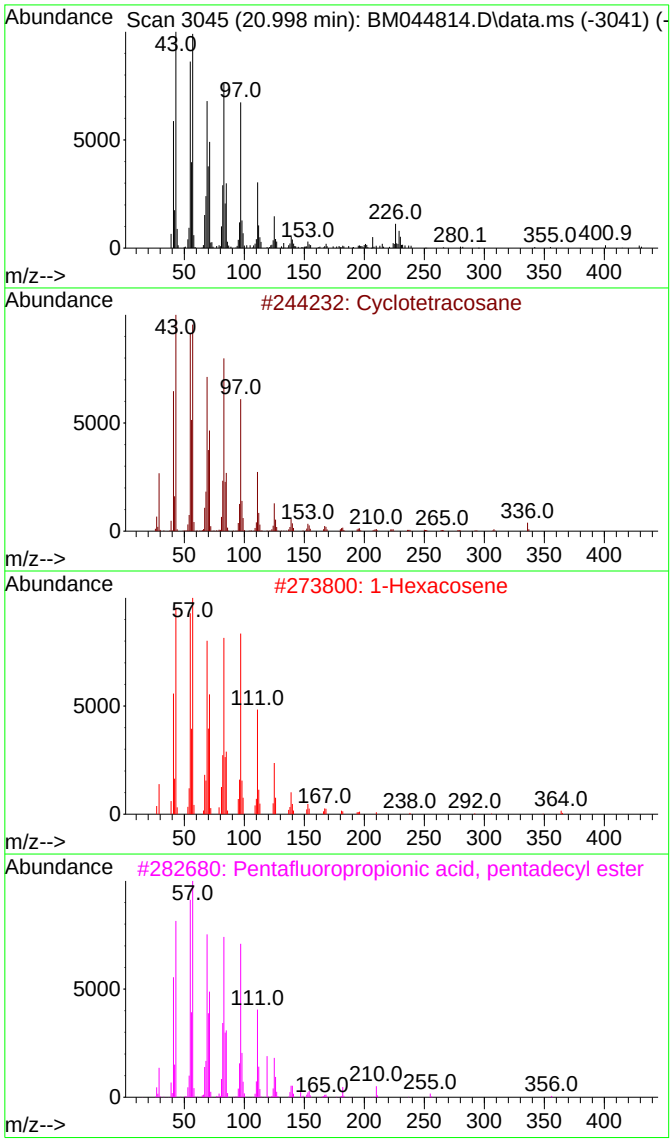
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

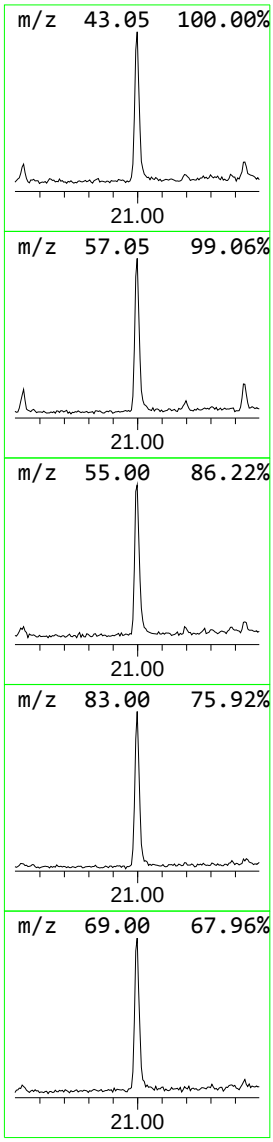
****

Peak Number 5 Cyclotetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.998	4.26 ng	342015	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	95
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4	Nonacos-1-ene	406	C29H58	018835-35-3	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044814.D
Acq On : 29 Mar 2024 13:11
Operator : MA/JU
Sample : P1879-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-01(2-4)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

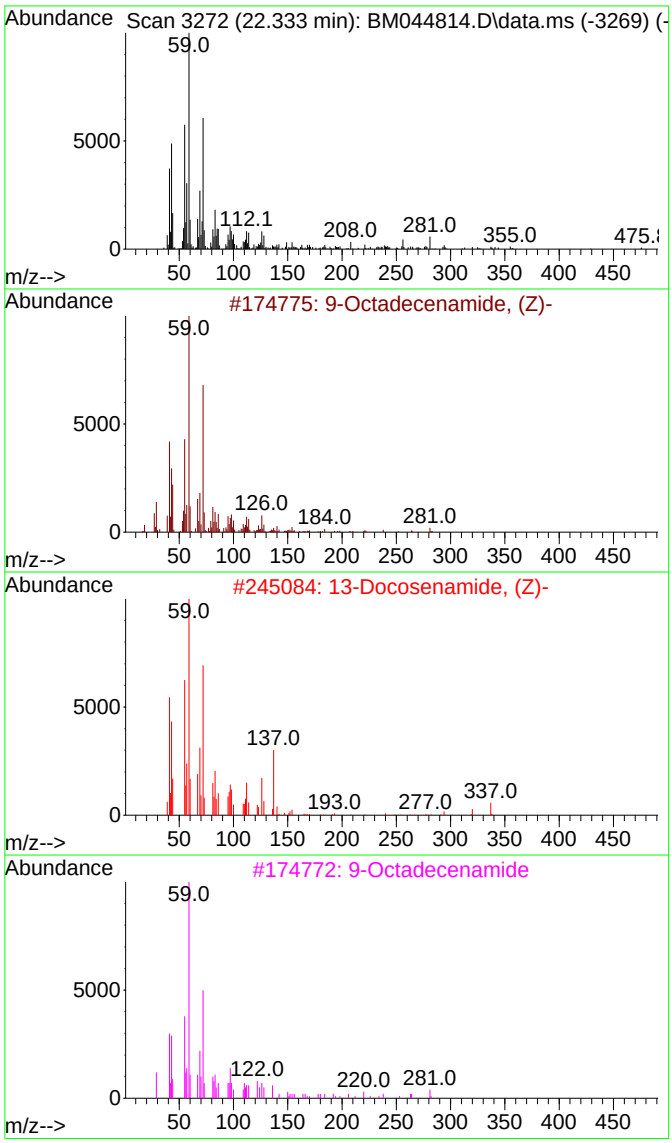
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

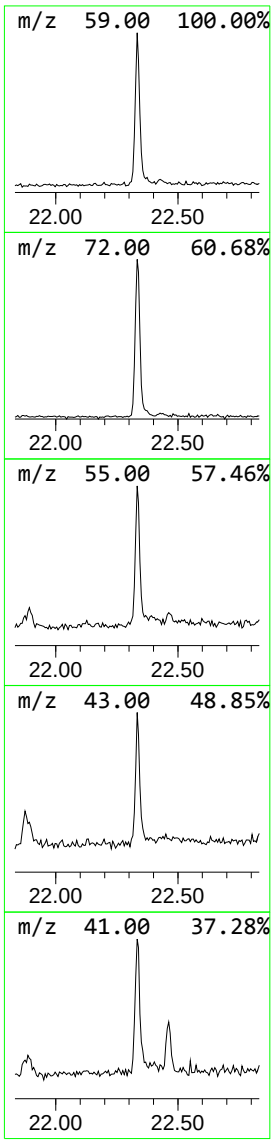
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.333	3.12 ng	250214	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	83
3	9-Octadecenamide	281	C18H35NO	003322-62-1	74
4	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64
5	Palmitoleamide	253	C16H31NO	106010-22-4	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032924\
Data File : BM044814.D
Acq On : 29 Mar 2024 13:11
Operator : MA/JU
Sample : P1879-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-01(2-4)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032824.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
Propylene Glycol	3.499	2.7	ng	84163	1	7.663	623472	20.0
n-Hexadecanoic ...	17.980	15.7	ng	879413	4	17.069	1118170	20.0
Cyclohexadecane	18.845	9.5	ng	530410	4	17.069	1118170	20.0
Octadecanoic acid	19.268	5.0	ng	402038	5	21.268	1605010	20.0
Cyclotetracosane	20.998	4.3	ng	342015	5	21.268	1605010	20.0
9-Octadecenamid...	22.333	3.1	ng	250214	5	21.268	1605010	20.0