LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032324\
Data File : BM044747.D
Acq On : 22 Mar 2024 22:40
Operator : MA/JU
Sample : P1831-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-01-032124

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-BM031324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM044747.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.975	144	151	163	rVB	80206	190901	3.27%	0.445%
2	5.311	371	378	386	rBV	2588555	4303776	73.78%	10.025%
3	5.722	442	448	456	rBV2	59785	113433	1.94%	0.264%
4	6.869	635	643	658	rBV	2564868	4248181	72.83%	9.895%
5	7.346	718	724	730	rBV4	27447	61850	1.06%	0.144%
6	7.687	773	782	789	rBV	816881	1326107	22.74%	3.089%
7	8.046	836	843	851	rBV2	33347	63619	1.09%	0.148%
8	8.846	972	979	994	rBV	1580937	2655572	45.53%	6.186%
9	10.463	1245	1254	1260	rBV	978872	1635172	28.03%	3.809%
10	12.134	1533	1538	1549	rBV3	40853	124330	2.13%	0.290%
11	12.945	1666	1676	1693	rBV	3323839	5046870	86.52%	11.756%
12	13.145	1701	1710	1718	rVB	46886	79067	1.36%	0.184%
13	14.234	1888	1895	1898	rBV	55470	75751	1.30%	0.176%
14	14.328	1898	1911	1918	rBV	1252478	1826406	31.31%	4.254%
15	15.192	2054	2058	2062	rVB	66694	87166	1.49%	0.203%
16	15.828	2158	2166	2173	rBV	2259058	3364188	57.68%	7.836%
17	16.057	2200	2205	2212	rBV	99280	182735	3.13%	0.426%
18	16.598	2293	2297	2302	rBV	101394	141142	2.42%	0.329%
19	16.851	2336	2340	2344	rBV	98637	117472	2.01%	0.274%
20	16.904	2345	2349	2356	rVB	45423	78452	1.34%	0.183%
21	17.080	2373	2379	2385	rBV	1294760	1870050	32.06%	4.356%
22	17.592	2462	2466	2471	rBV	115211	137690	2.36%	0.321%
23	17.874	2508	2514	2520	rBV2	173452	363063	6.22%	0.846%
24	17.998	2530	2535	2549	rVB	677382	975988	16.73%	2.273%
25	18.286	2580	2584	2589	rBV	143702	185647	3.18%	0.432%
26	18.757	2661	2664	2668	rBV3	39127	66478	1.14%	0.155%
27	18.927	2689	2693	2699	rBV	215266	291240	4.99%	0.678%
28	19.151	2726	2731	2736	rBV	186937	347856	5.96%	0.810%
29	19.280	2749	2753	2761	rBV2	215680	406492	6.97%	0.947%
30	19.510	2789	2792	2797	rBV	348137	400424	6.86%	0.933%
31	19.727	2823	2829	2841	rVB	4606603	5832870	100.00%	13.586%
32	20.051	2880	2884	2887	rBV	298695	322483	5.53%	0.751%
33	20.551	2965	2969	2972	rBV	294400	351626	6.03%	0.819%
34	21.010	3044	3047	3051	rBV	582387	691040	11.85%	1.610%
35	21.280	3088	3093	3098	rBV	1589310	2211149	37.91%	5.150%
36	21.451	3120	3122	3126	rVB	253542	243613	4.18%	0.567%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032324\
Data File : BM044747.D
Acq On : 22 Mar 2024 22:40
Operator : MA/JU
Sample : P1831-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-01-032124

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-BM031324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.892	3194	3197	3207	rVB2	304359	517947	8.88%	1.206%
38	23.521	3469	3474	3481	rVB	1077762	1993550	34.18%	4.644%

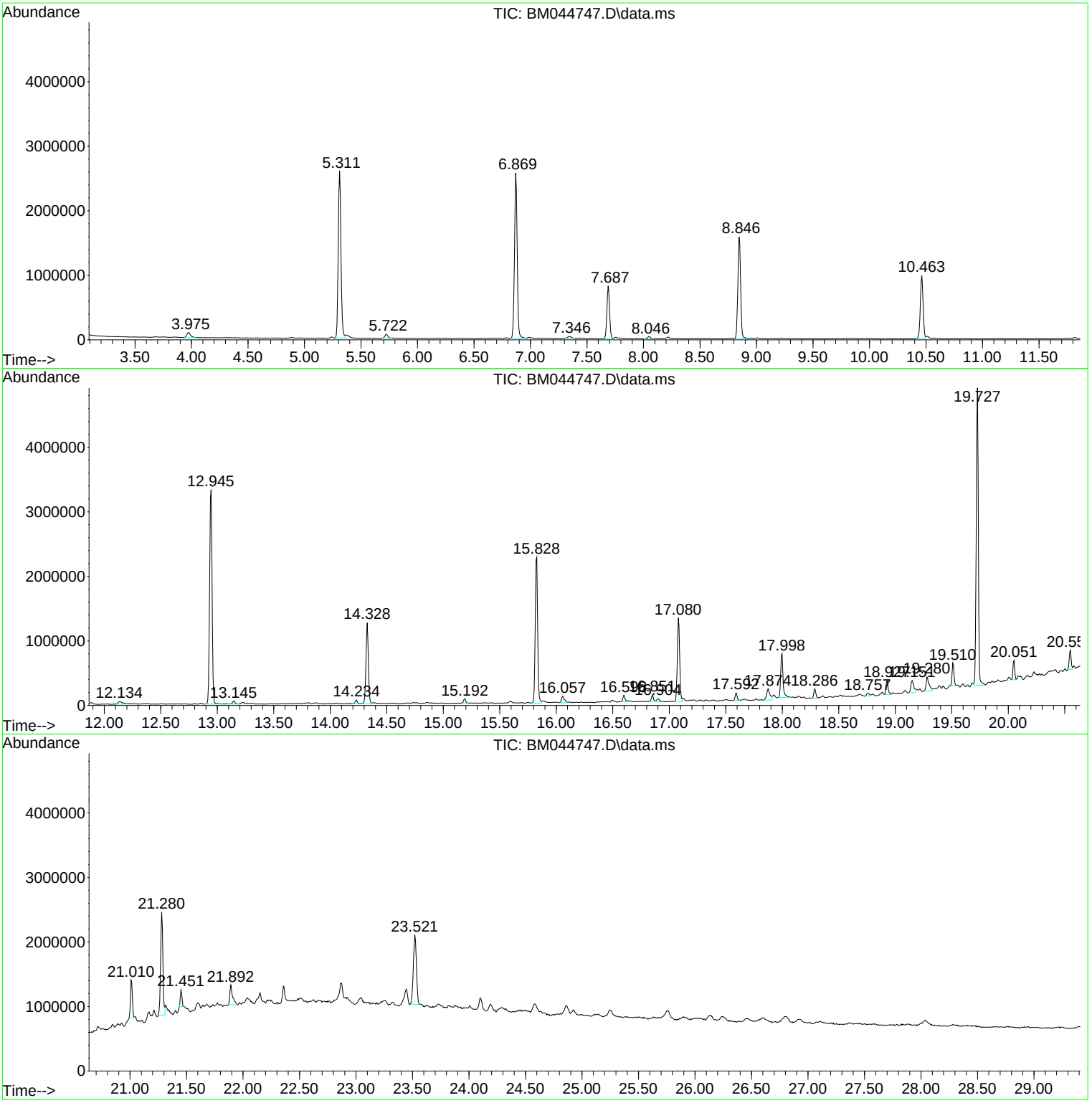
Sum of corrected areas: 42931396

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032324\
Data File : BM044747.D
Acq On : 22 Mar 2024 22:40
Operator : MA/JU
Sample : P1831-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-01-032124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.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\BM032324\
Data File : BM044747.D
Acq On : 22 Mar 2024 22:40
Operator : MA/JU
Sample : P1831-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-01-032124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

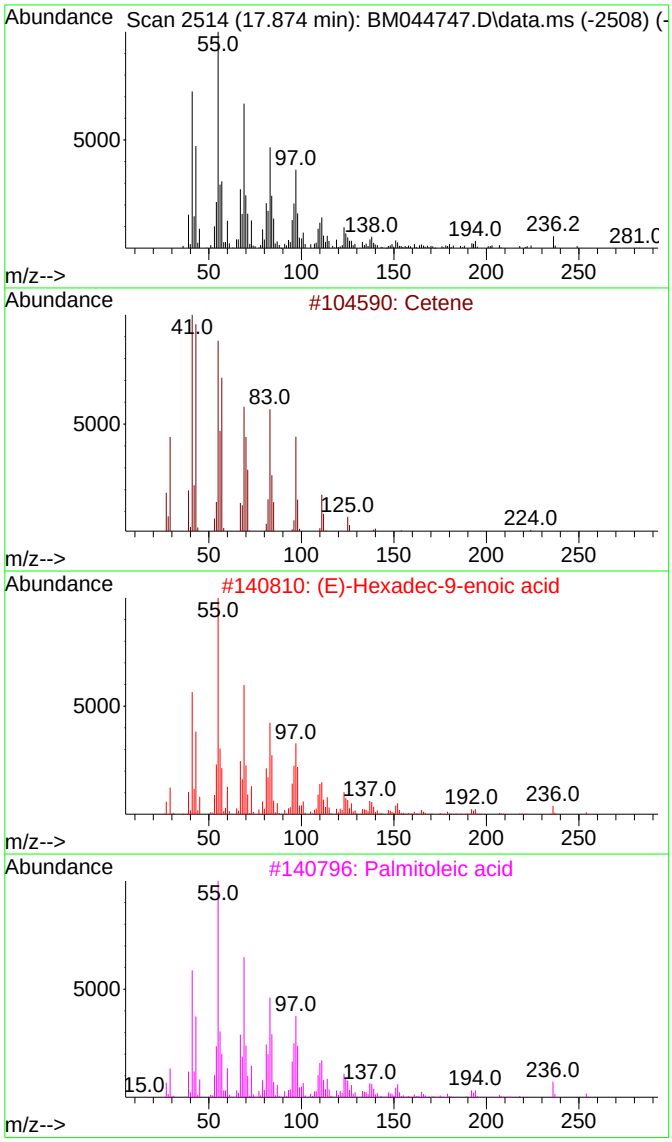
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

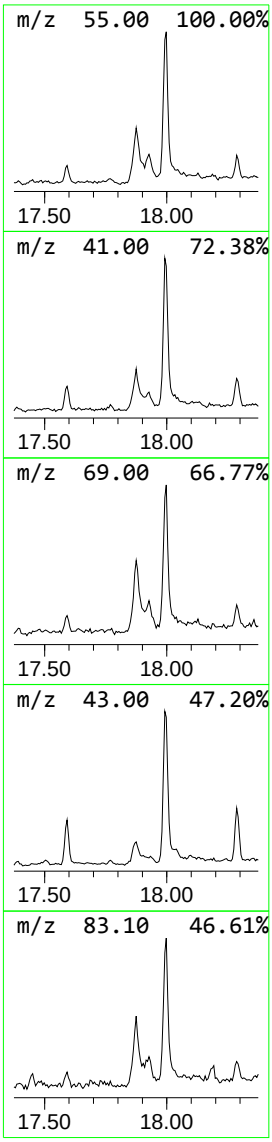
****

Peak Number 2 Cetene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.874	3.88 ng	363063	Phenanthrene-d10	17.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	96
2	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	87
3	Palmitoleic acid	254	C16H30O2	000373-49-9	87
4	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	74
5	Cyclopropane, nonyl-	168	C12H24	074663-85-7	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032324\
Data File : BM044747.D
Acq On : 22 Mar 2024 22:40
Operator : MA/JU
Sample : P1831-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-01-032124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

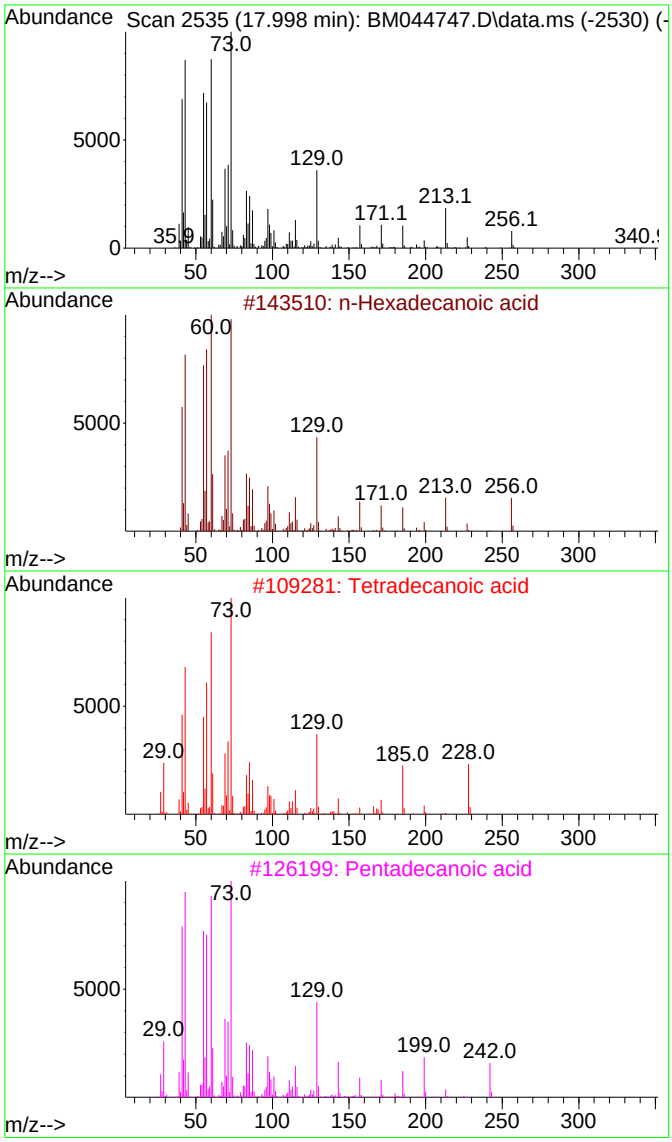
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

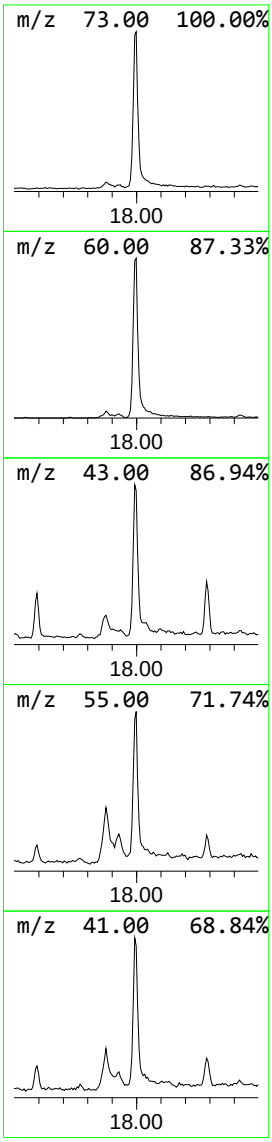
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.998	10.44 ng	975988	Phenanthrene-d10	17.080

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	90
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032324\
Data File : BM044747.D
Acq On : 22 Mar 2024 22:40
Operator : MA/JU
Sample : P1831-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-01-032124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

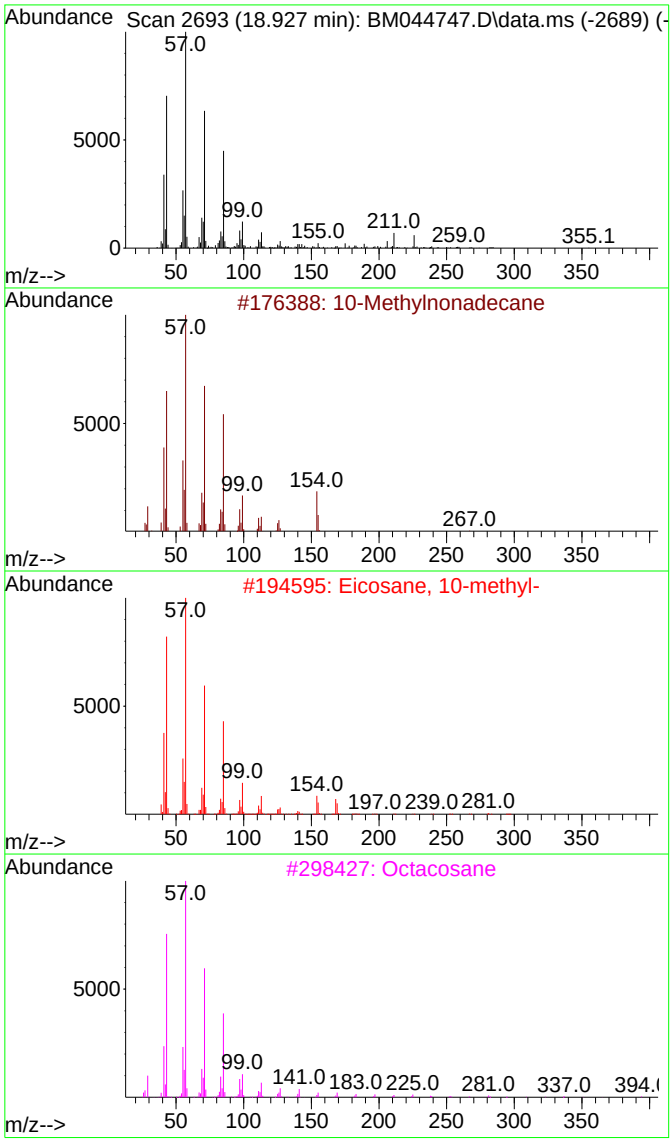
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

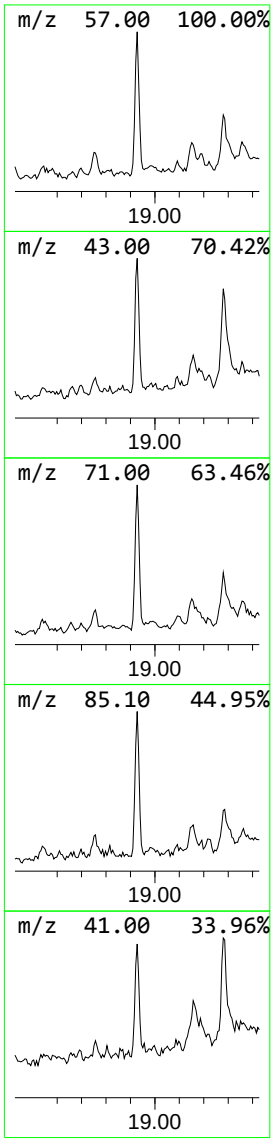
****

Peak Number 4 10-Methylnonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.927	3.11 ng	291240	Phenanthrene-d10	17.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Methylnonadecane	282	C20H42	056862-62-5	87
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	87
3	Octacosane	394	C28H58	000630-02-4	86
4	Hexadecane	226	C16H34	000544-76-3	81
5	Tetradecane	198	C14H30	000629-59-4	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032324\
Data File : BM044747.D
Acq On : 22 Mar 2024 22:40
Operator : MA/JU
Sample : P1831-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-01-032124

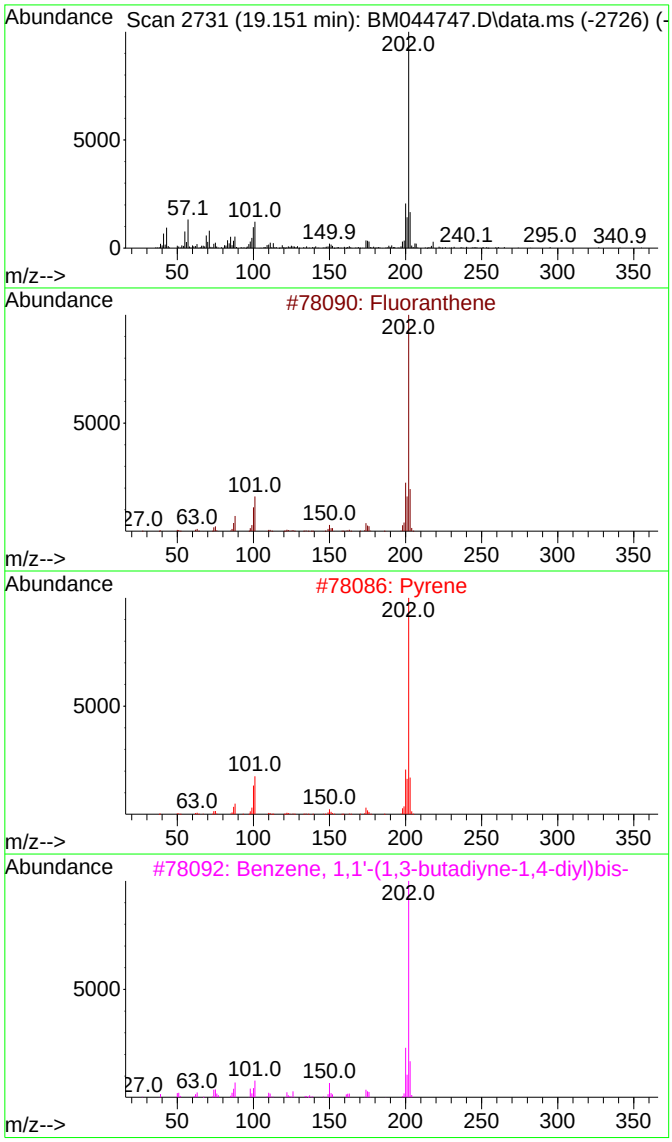
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

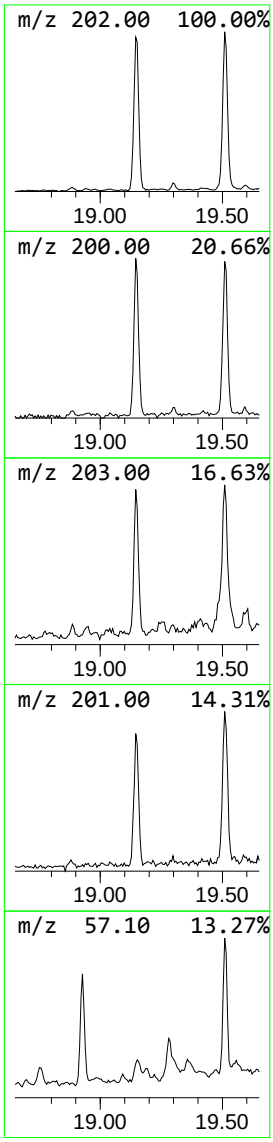
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.151	3.72 ng	347856	Phenanthrene-d10	17.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	97
2	Pyrene	202	C16H10	000129-00-0	94
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	76
4	1,4-Pentadiyn-3-one, 1,5-diphenyl-	230	C17H10O	015814-30-9	56
5	7H-Furo[3,2-g][1]benzopyran-7-on...	202	C11H6O4	002009-24-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032324\
Data File : BM044747.D
Acq On : 22 Mar 2024 22:40
Operator : MA/JU
Sample : P1831-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-01-032124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

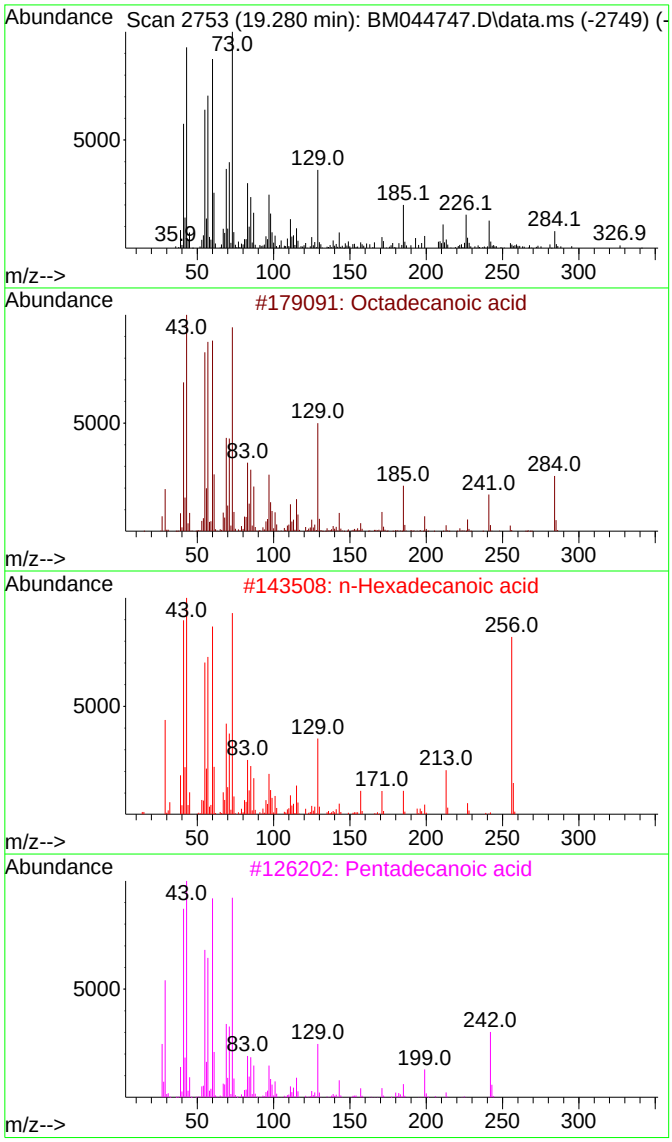
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

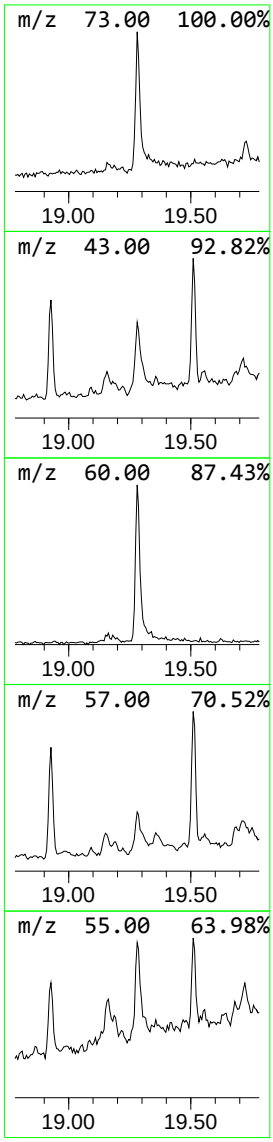
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.280	3.68 ng	406492	Chrysene-d12	21.280

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032324\
Data File : BM044747.D
Acq On : 22 Mar 2024 22:40
Operator : MA/JU
Sample : P1831-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-01-032124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

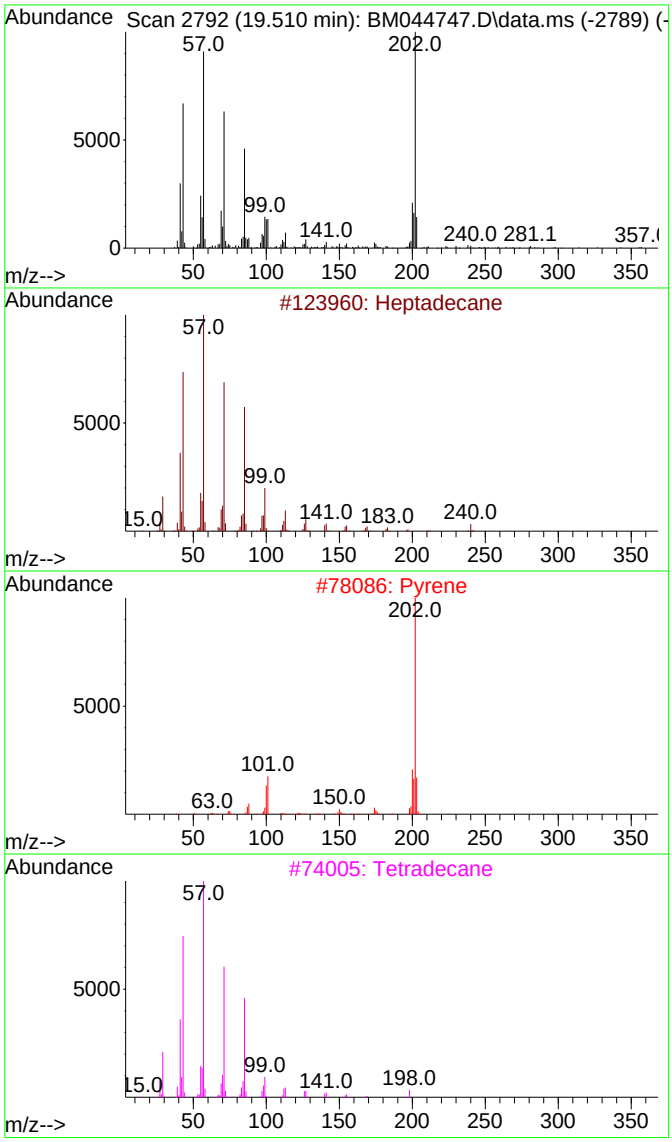
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

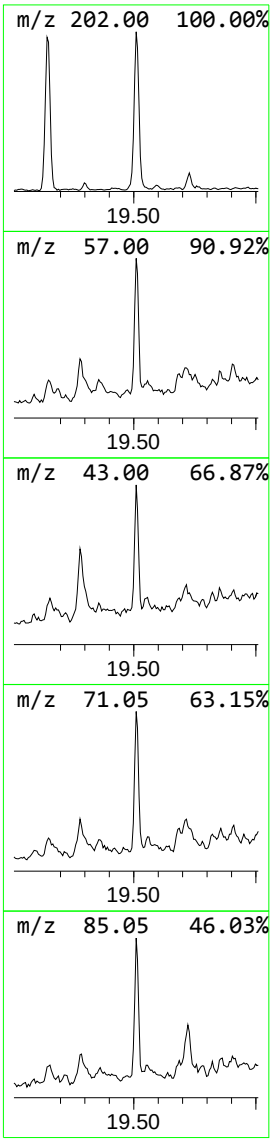
****

Peak Number 7 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.510	3.62 ng	400424	Chrysene-d12	21.280

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Pyrene	202	C16H10	000129-00-0	46
3	Tetradecane	198	C14H30	000629-59-4	42
4	Fluoranthene	202	C16H10	000206-44-0	41
5	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032324\
Data File : BM044747.D
Acq On : 22 Mar 2024 22:40
Operator : MA/JU
Sample : P1831-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-01-032124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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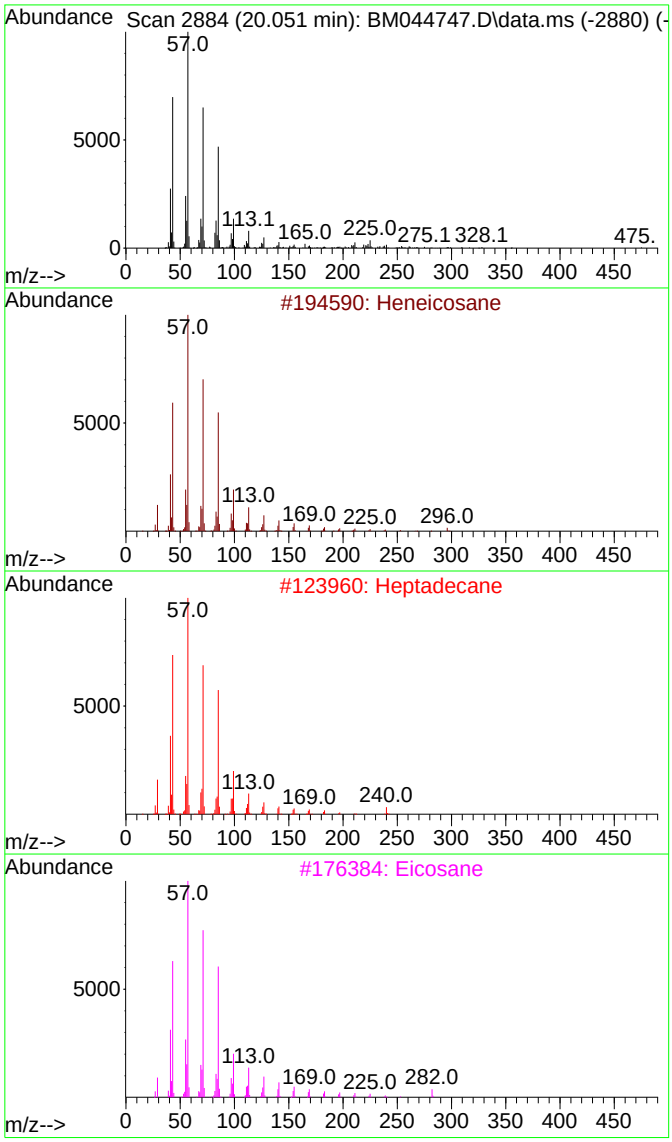
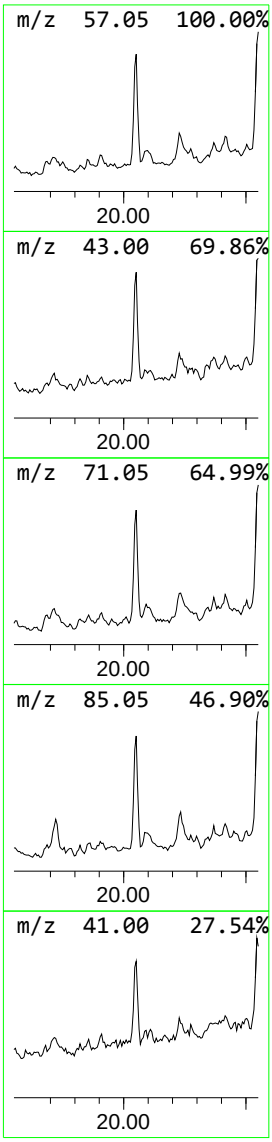
Peak Number 8 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.051	2.92 ng	322483	Chrysene-d12	21.280

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Heptadecane	240	C17H36	000629-78-7	95
3	Eicosane	282	C20H42	000112-95-8	95
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
5	Decane, 1-iodo-	268	C10H21I	002050-77-3	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032324\
Data File : BM044747.D
Acq On : 22 Mar 2024 22:40
Operator : MA/JU
Sample : P1831-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-01-032124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

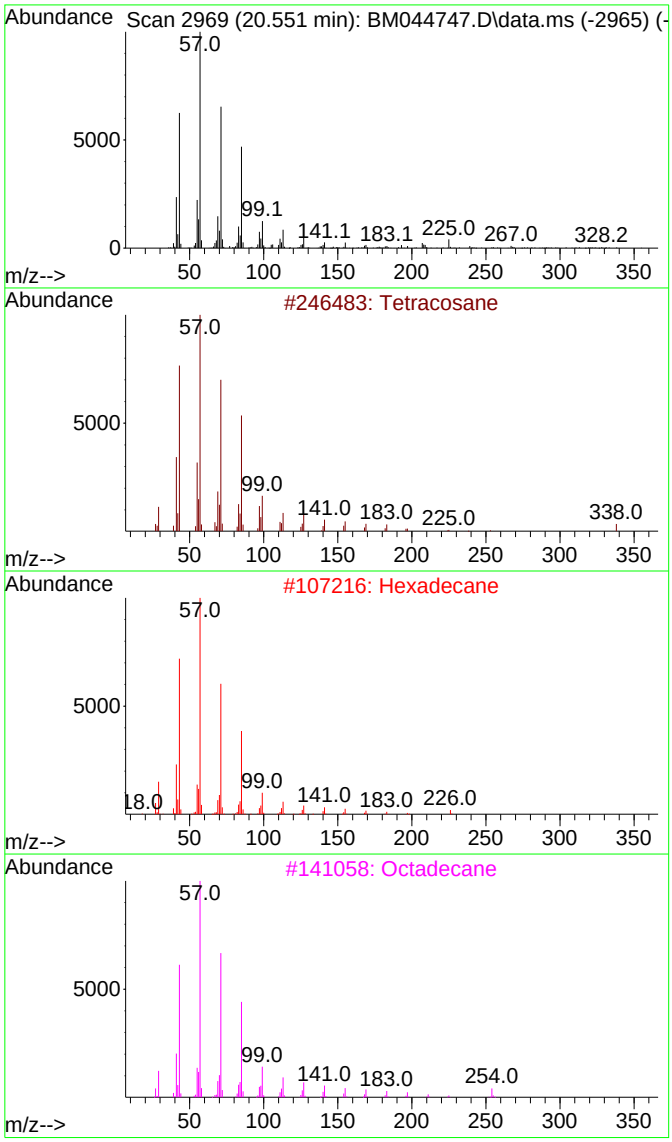
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

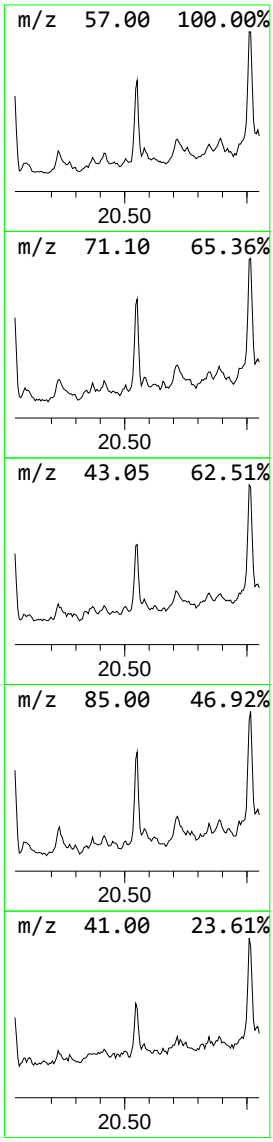
****

Peak Number 9 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.551	3.18 ng	351626	Chrysene-d12	21.280

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	98
2	Hexadecane	226	C16H34	000544-76-3	95
3	Octadecane	254	C18H38	000593-45-3	94
4	Hexacosane	366	C26H54	000630-01-3	91
5	Heptacosane	380	C27H56	000593-49-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032324\
Data File : BM044747.D
Acq On : 22 Mar 2024 22:40
Operator : MA/JU
Sample : P1831-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-01-032124

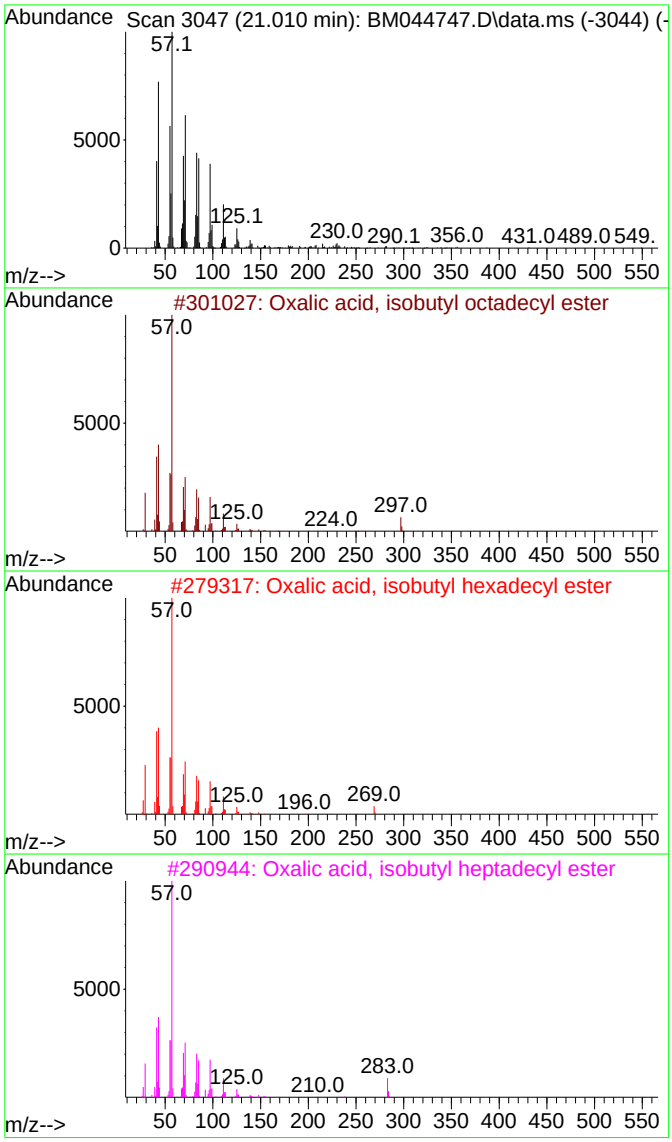
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

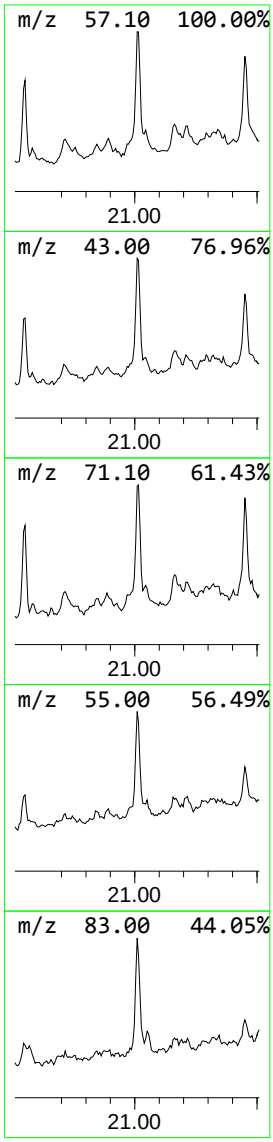
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Oxalic acid, isobutyl octad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.009	6.25 ng	691040	Chrysene-d12	21.280

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
2	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
3	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	91
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87
5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	87





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Acq On : 22 Mar 2024 22:40
Operator : MA/JU
Sample : P1831-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-01-032124

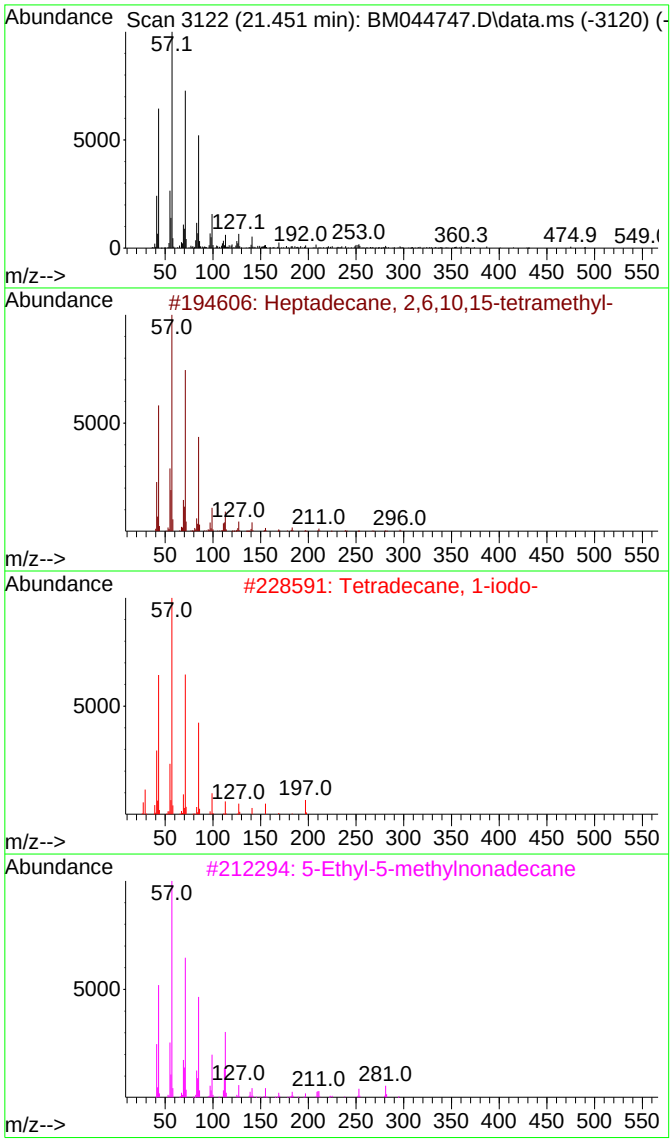
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

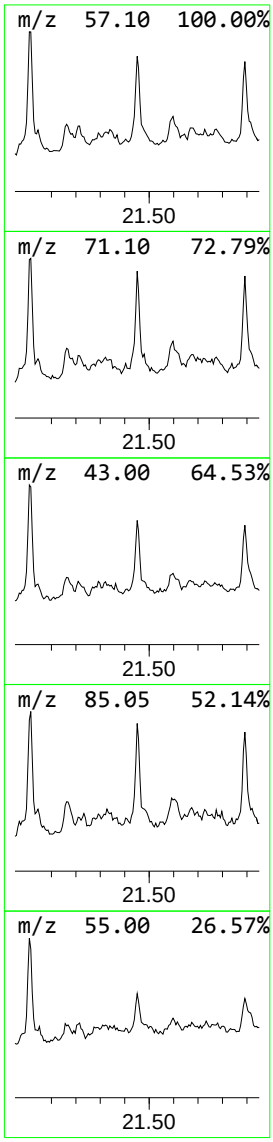
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Heptadecane, 2,6,10,15-tetr... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.451	2.20 ng	243613	Chrysene-d12	21.280

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
2	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
3	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	80
4	Nonadecane	268	C19H40	000629-92-5	80
5	Eicosane	282	C20H42	000112-95-8	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032324\
Data File : BM044747.D
Acq On : 22 Mar 2024 22:40
Operator : MA/JU
Sample : P1831-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-01-032124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

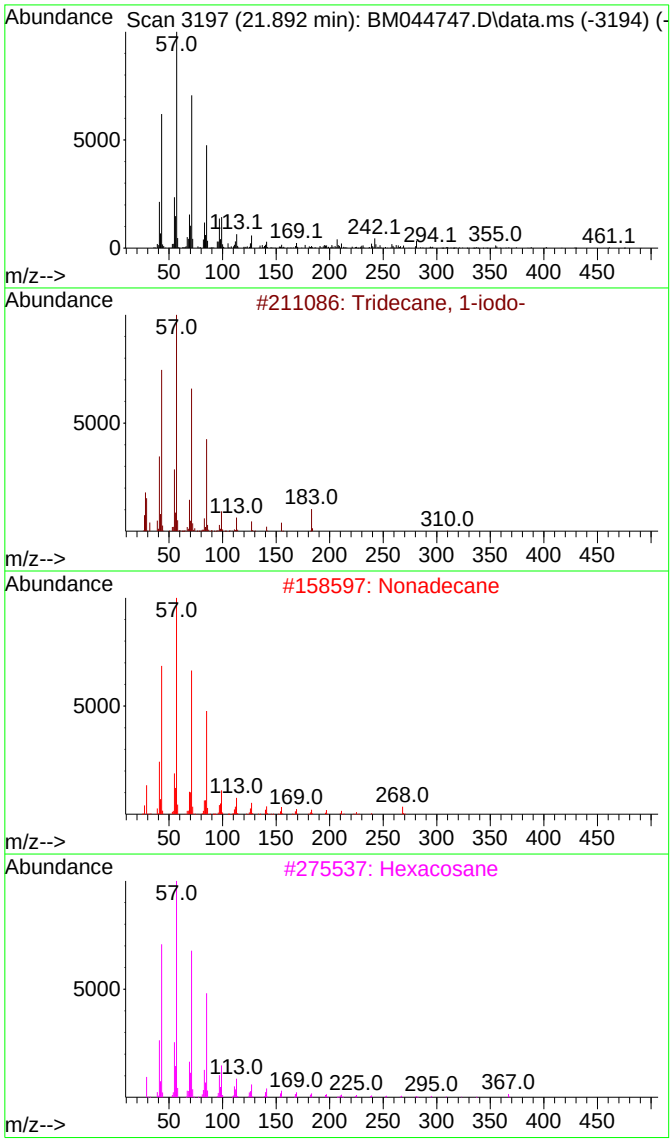
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

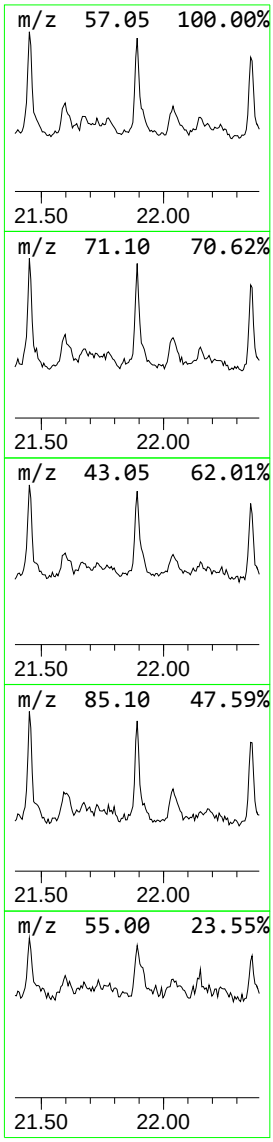
****

Peak Number 12 Tridecane, 1-iodo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.892	4.68 ng	517947	Chrysene-d12	21.280

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
2	Nonadecane	268	C19H40	000629-92-5	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	87
5	Octacosane	394	C28H58	000630-02-4	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032324\
Data File : BM044747.D
Acq On : 22 Mar 2024 22:40
Operator : MA/JU
Sample : P1831-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CL-01-032124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.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
Cetene	17.874	3.9	ng	363063	4	17.080	1870050	20.0
n-Hexadecanoic ...	17.998	10.4	ng	975988	4	17.080	1870050	20.0
10-Methylnonade...	18.927	3.1	ng	291240	4	17.080	1870050	20.0
Benzene, 1,1'-(...	19.151	3.7	ng	347856	4	17.080	1870050	20.0
Octadecanoic acid	19.280	3.7	ng	406492	5	21.280	2211150	20.0
Heptadecane	19.510	3.6	ng	400424	5	21.280	2211150	20.0
Heneicosane	20.051	2.9	ng	322483	5	21.280	2211150	20.0
Tetracosane	20.551	3.2	ng	351626	5	21.280	2211150	20.0
Oxalic acid, is...	21.009	6.3	ng	691040	5	21.280	2211150	20.0
Heptadecane, 2,...	21.451	2.2	ng	243613	5	21.280	2211150	20.0
Tridecane, 1-iodo-	21.892	4.7	ng	517947	5	21.280	2211150	20.0