LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021324\
Data File : BP019684.D
Acq On : 13 Feb 2024 18:50
Operator : MA/JU
Sample : P1453-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-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_P\Methods\8270E-BP013124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP019684.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.628	88	92	101	rBV	41776	64225	1.08%	0.235%
2	5.022	323	329	337	rVB	96899	144475	2.42%	0.529%
3	5.475	399	406	418	rBV	1431840	2216266	37.16%	8.121%
4	7.075	670	678	689	rBV	1423535	2328719	39.04%	8.533%
5	7.905	811	819	825	rBV	274595	458386	7.68%	1.680%
6	9.075	1008	1018	1027	rBV	889104	1544232	25.89%	5.658%
7	10.704	1286	1295	1303	rBV	339057	590410	9.90%	2.163%
8	13.163	1706	1713	1733	rBV	2292324	3548457	59.49%	13.002%
9	14.534	1938	1946	1954	rBV	518121	819029	13.73%	3.001%
10	16.034	2193	2201	2220	rBV	2251696	3496661	58.62%	12.812%
11	17.292	2408	2415	2420	rBV	714711	1062139	17.81%	3.892%
12	17.333	2420	2422	2428	rVB	58947	77370	1.30%	0.283%
13	18.192	2563	2568	2577	rBV	418909	580967	9.74%	2.129%
14	19.304	2752	2757	2763	rBV	92471	141807	2.38%	0.520%
15	19.427	2774	2778	2785	rBV	166799	231931	3.89%	0.850%
16	19.657	2813	2817	2820	rVB	60314	75358	1.26%	0.276%
17	19.863	2846	2852	2858	rBV	4927974	5964890	100.00%	21.856%
18	20.545	2964	2968	2974	rVB	232698	280210	4.70%	1.027%
19	20.616	2976	2980	2984	rBV	234743	290517	4.87%	1.064%
20	20.657	2985	2987	2992	rVB	52956	66515	1.12%	0.244%
21	21.110	3060	3064	3071	rBV2	294962	424207	7.11%	1.554%
22	21.386	3106	3111	3116	rBV	937805	1281808	21.49%	4.697%
23	21.563	3138	3141	3146	rVB	103972	128973	2.16%	0.473%
24	22.033	3218	3221	3228	rVB3	82764	132567	2.22%	0.486%
25	23.810	3516	3523	3531	rVB	612837	1341835	22.50%	4.917%

Sum of corrected areas: 27291954

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Misc :
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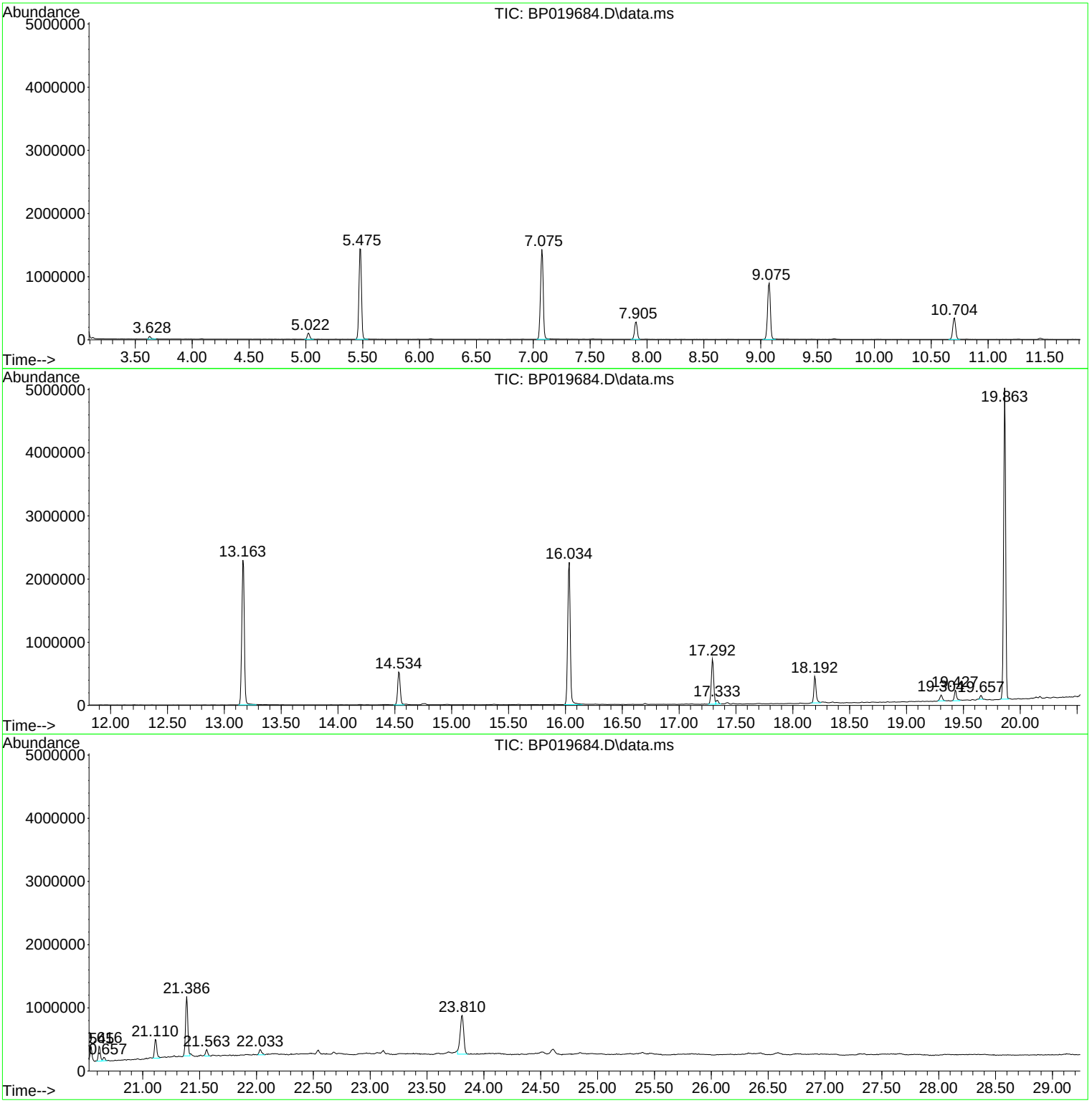
Instrument :
BNA_P
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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_P\Data\BP021324\
Data File : BP019684.D
Acq On : 13 Feb 2024 18:50
Operator : MA/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

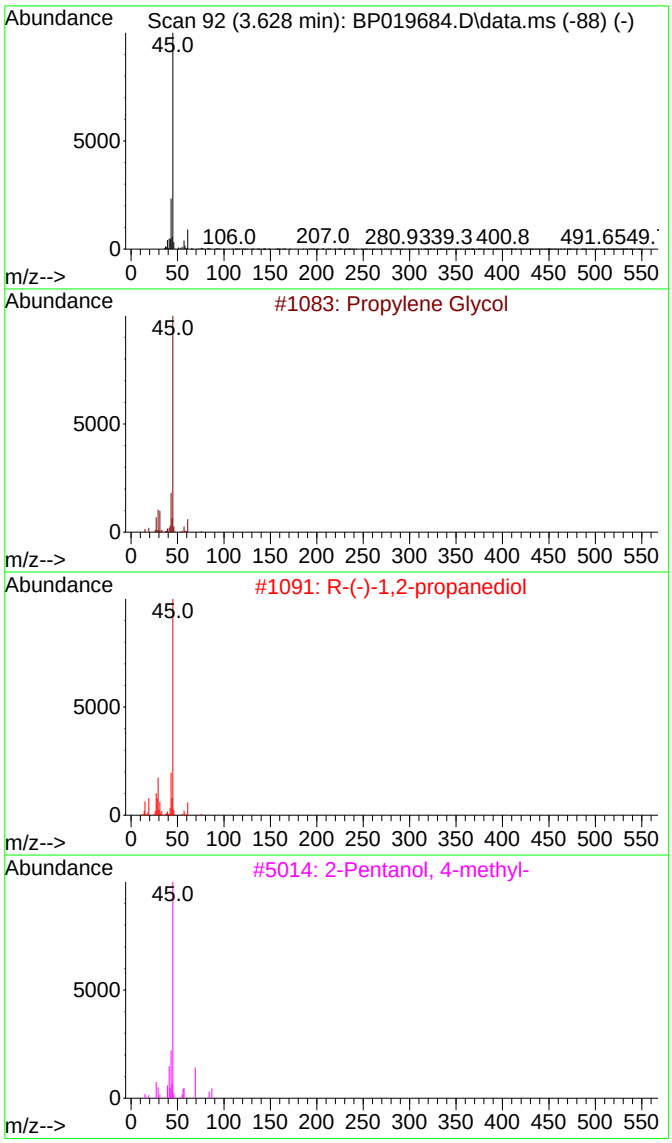
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

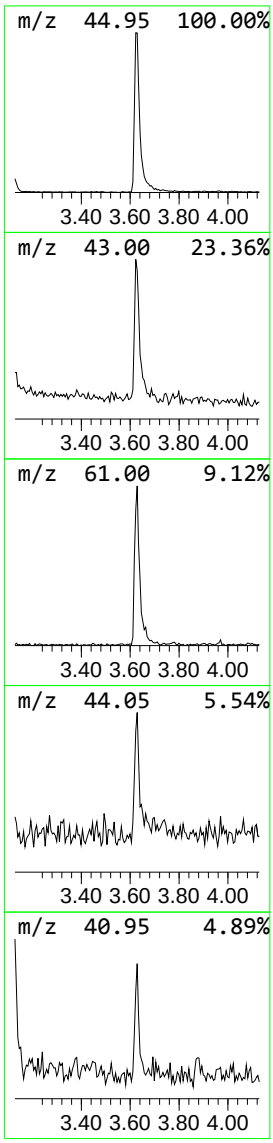
****

Peak Number 1 Propylene Glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.628	2.80 ng	64225	1,4-Dichlorobenzene-d4	7.905

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	72
3	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	39
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	2,4-Pentanediol	104	C5H12O2	000625-69-4	9





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Data File : BP019684.D
Acq On : 13 Feb 2024 18:50
Operator : MA/JU
Sample : P1453-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-3

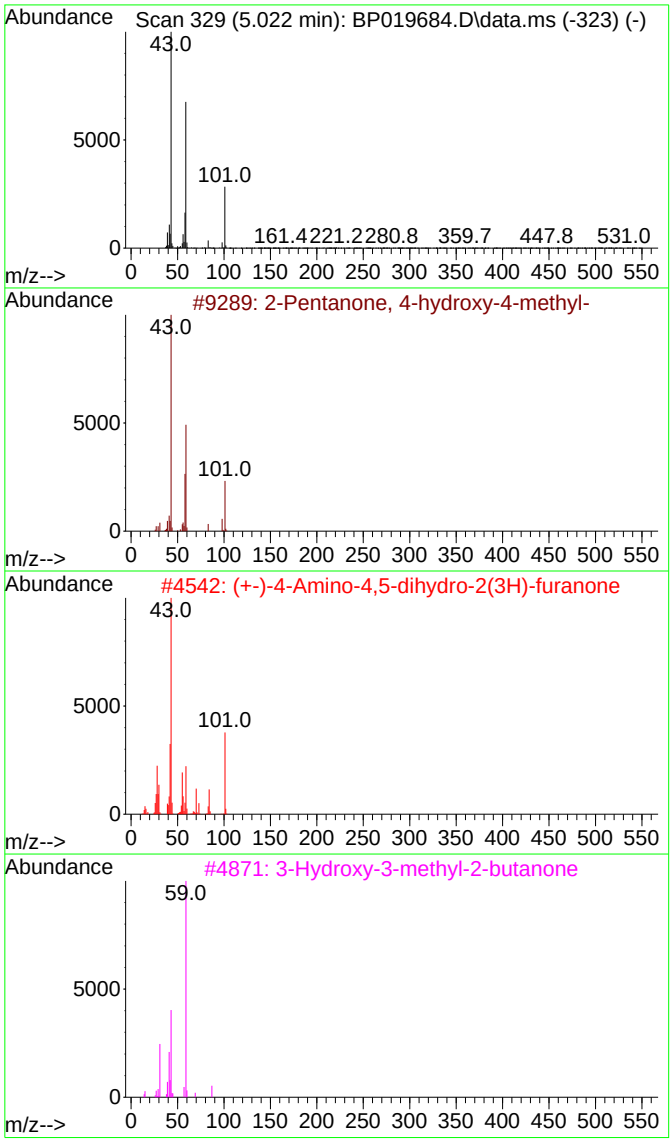
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

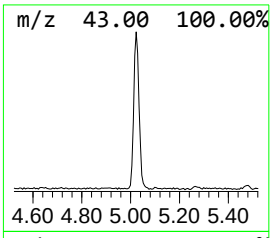
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

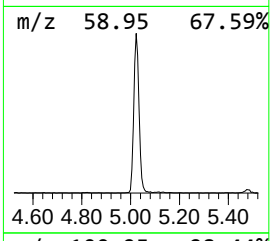
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

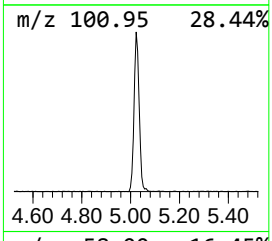
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	6.30 ng	144475	1,4-Dichlorobenzene-d4	7.905

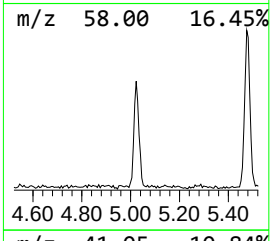
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	40
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10

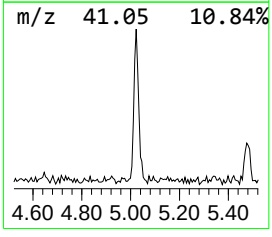












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021324\
Data File : BP019684.D
Acq On : 13 Feb 2024 18:50
Operator : MA/JU
Sample : P1453-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

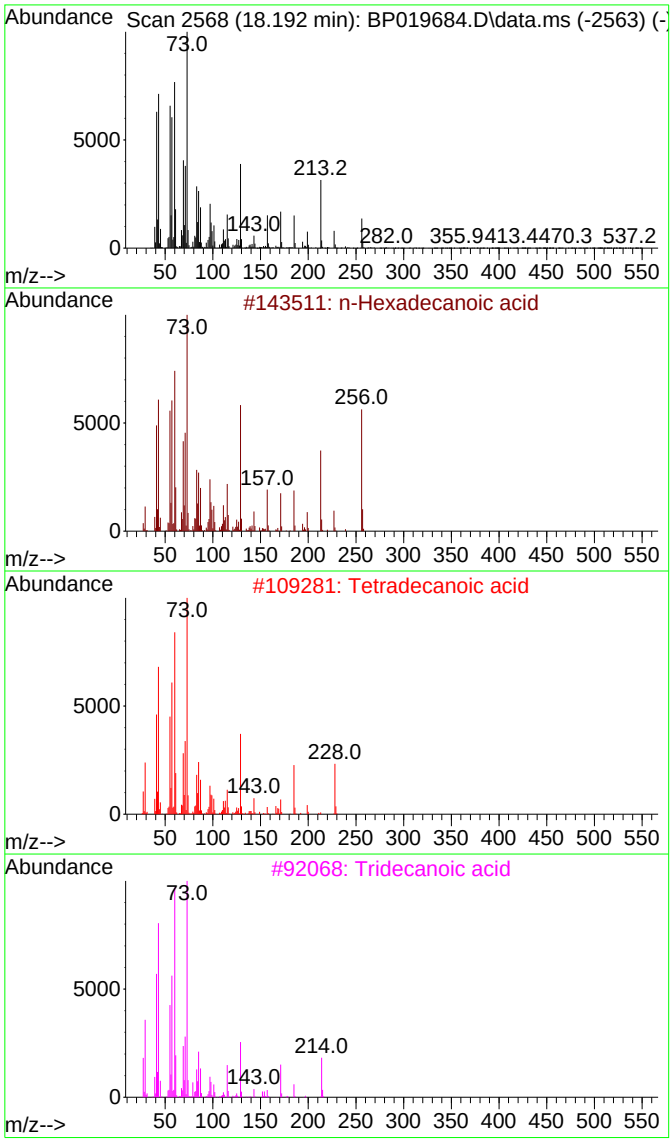
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

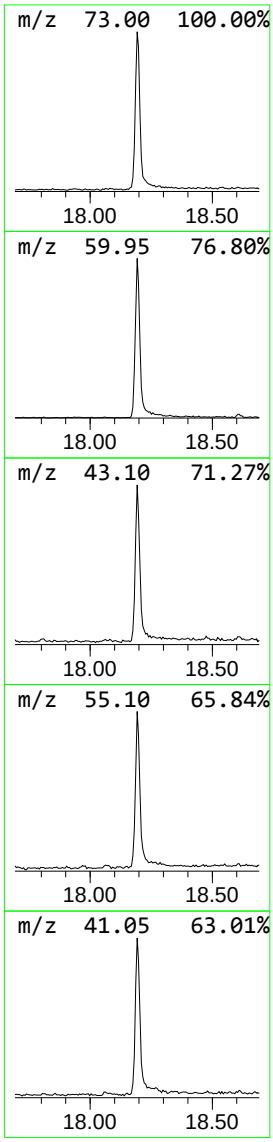
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	10.94 ng	580967	Phenanthrene-d10	17.292

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	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Octadecanoic acid	284	C18H36O2	000057-11-4	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021324\
Data File : BP019684.D
Acq On : 13 Feb 2024 18:50
Operator : MA/JU
Sample : P1453-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

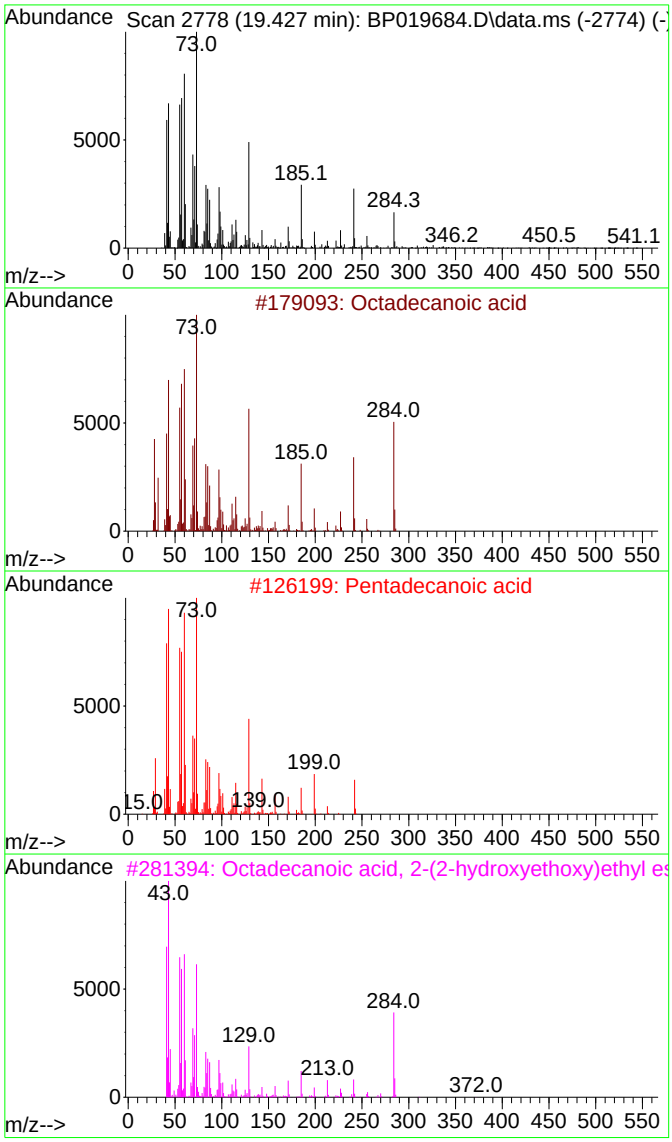
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

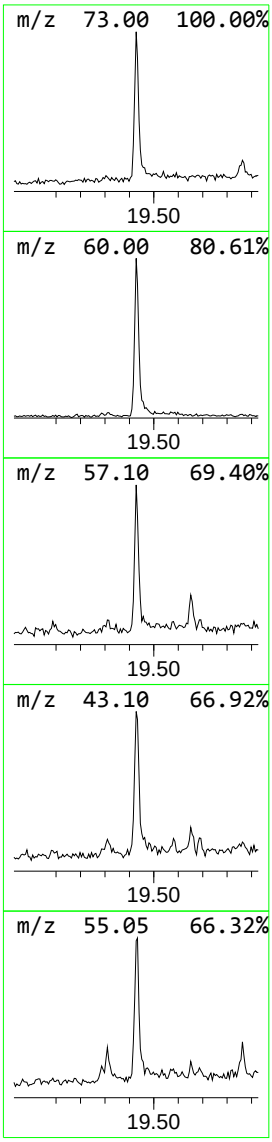
****

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.427	3.62 ng	231931	Chrysene-d12	21.386

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	91
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	90
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	87





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Data File : BP019684.D
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Operator : MA/JU
Sample : P1453-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

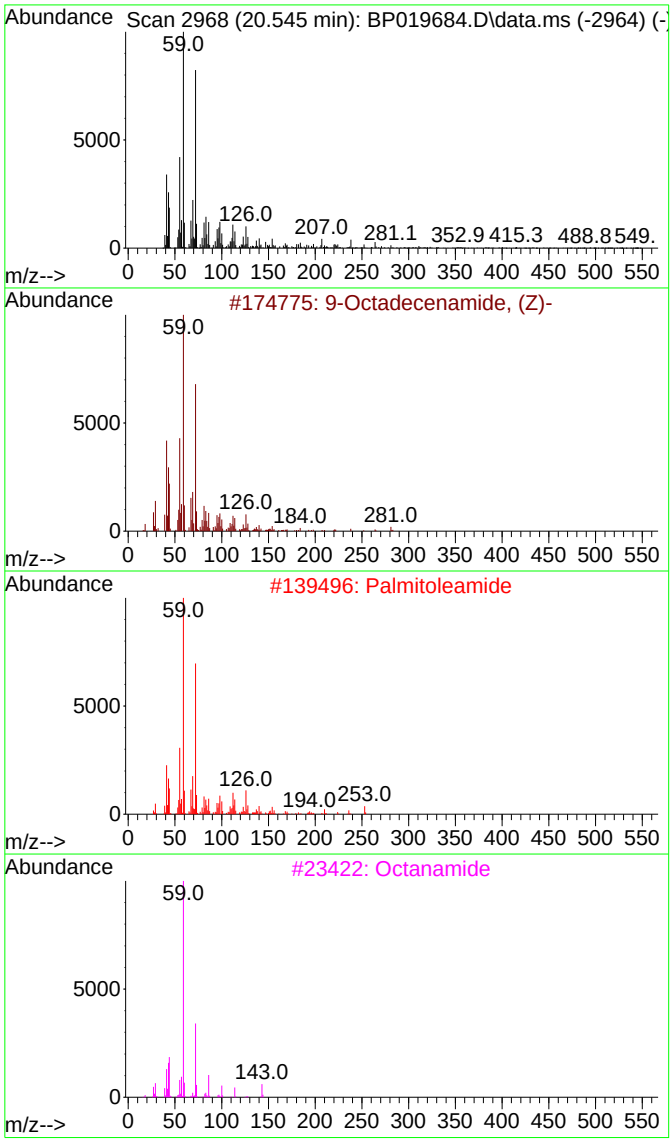
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

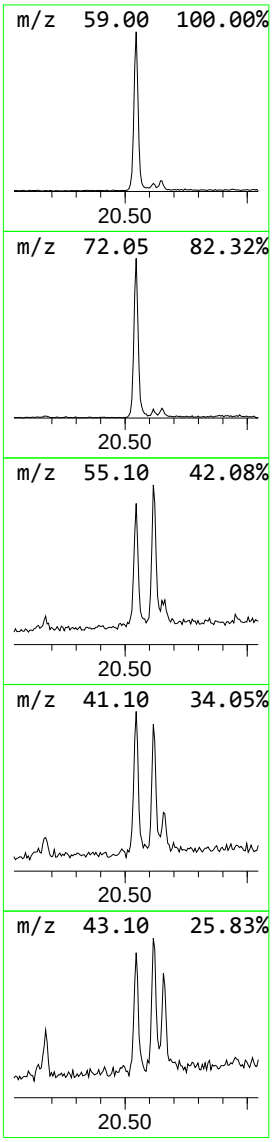
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.545	4.37 ng	280210	Chrysene-d12	21.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Palmitoleamide	253	C16H31NO	106010-22-4	53
3	Octanamide	143	C8H17NO	000629-01-6	43
4	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	43
5	Oxprenolol, trimethylsilyl ether	337	C18H31NO3Si	959016-76-3	30





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Data File : BP019684.D
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Operator : MA/JU
Sample : P1453-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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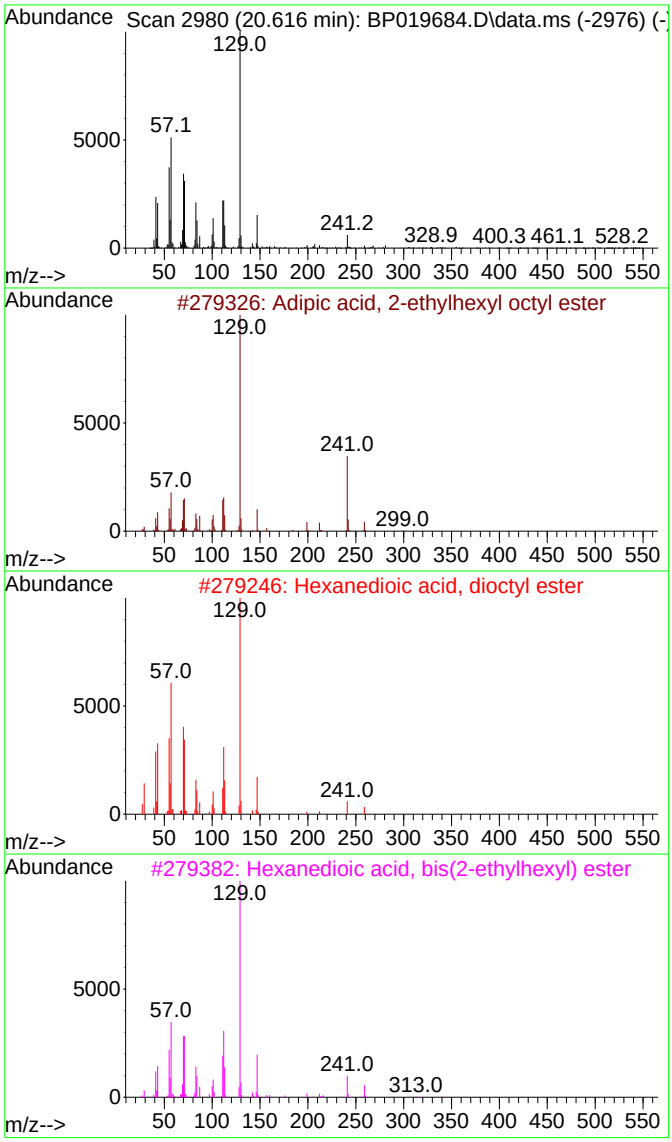
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

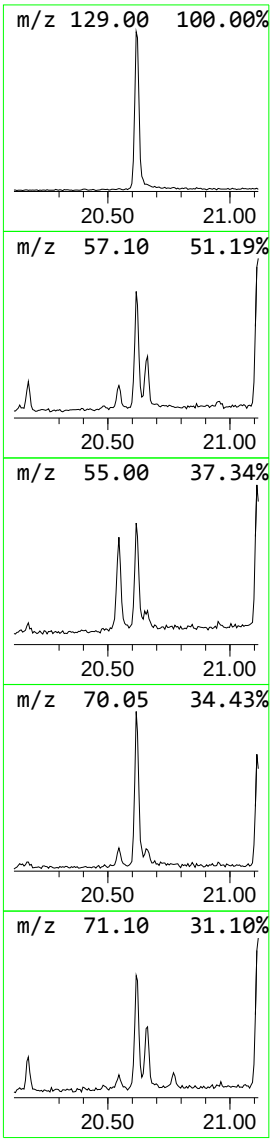
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Adipic acid, 2-ethylhexyl o... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.616	4.53 ng	290517	Chrysene-d12	21.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	91
2	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	87
3	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	87
4	Diisooctyl adipate	370	C22H42O4	001330-86-5	83
5	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	68





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Sample : P1453-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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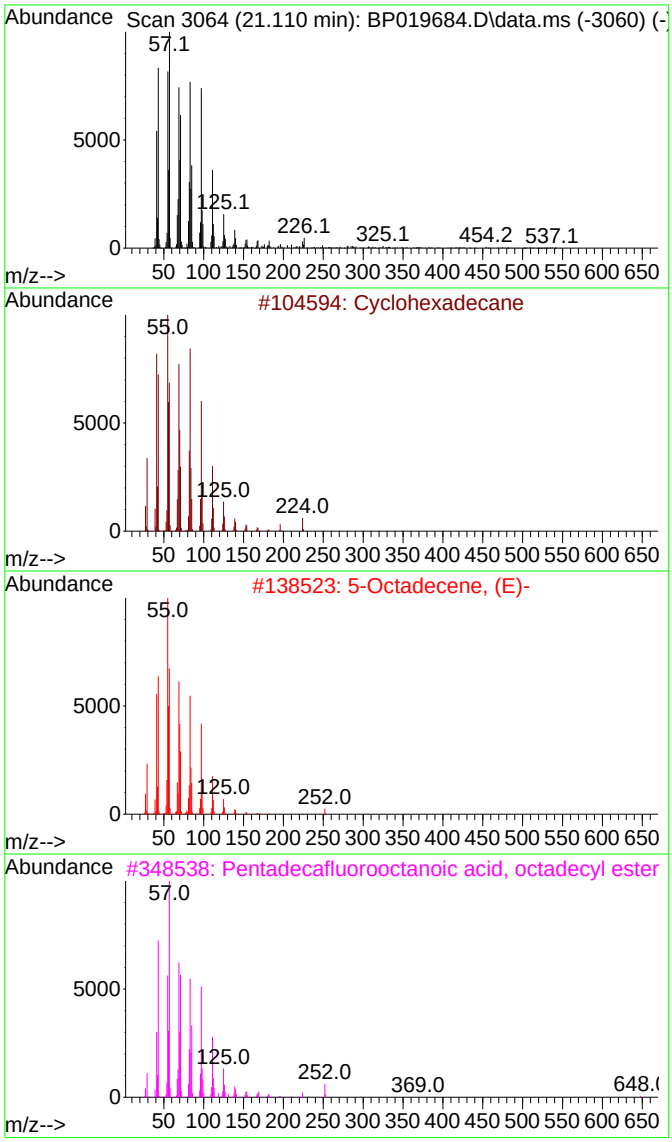
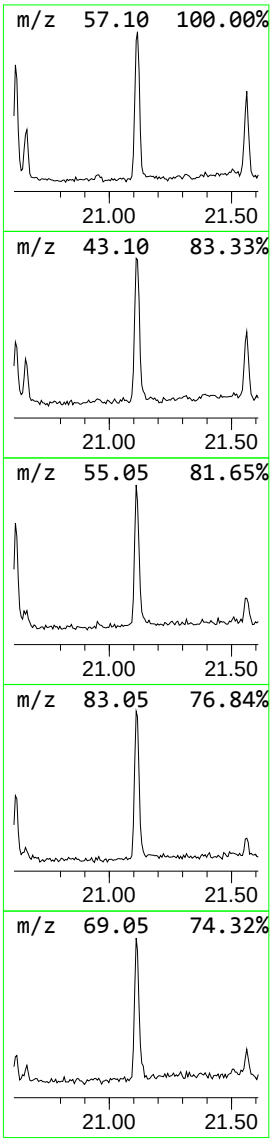
Peak Number 8 Cyclohexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.110	6.62 ng	424207	Chrysene-d12	21.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	97
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	1-Heptadecene	238	C17H34	006765-39-5	93





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BNA_P
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

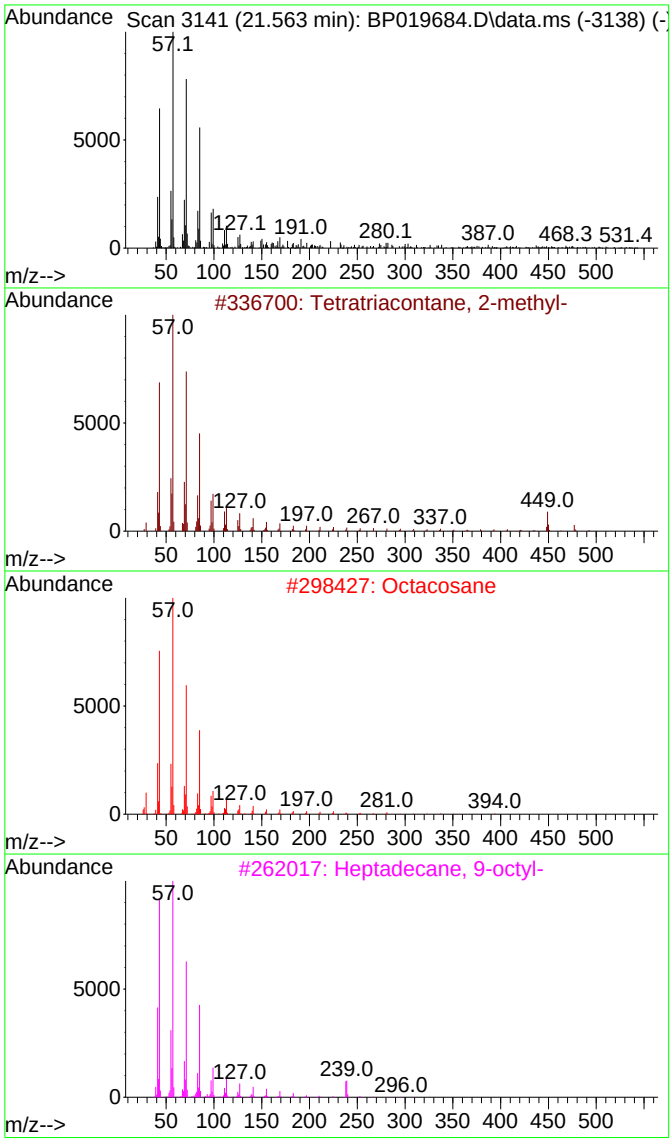
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

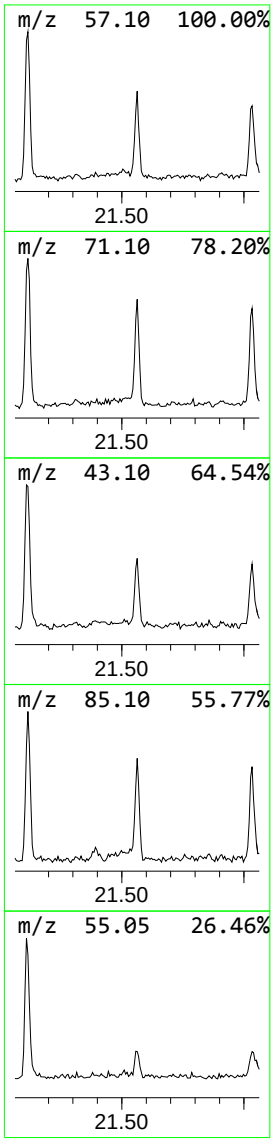
****

Peak Number 9 Tetratriacontane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.563	2.01 ng	128973	Chrysene-d12	21.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratriacontane, 2-methyl-	493	C35H72	014167-65-8	93
2	Octacosane	394	C28H58	000630-02-4	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Dotriacontane, 2-methyl-	465	C33H68	001720-11-2	87
5	Tricosane, 2-methyl-	338	C24H50	001928-30-9	87





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Data File : BP019684.D
Acq On : 13 Feb 2024 18:50
Operator : MA/JU
Sample : P1453-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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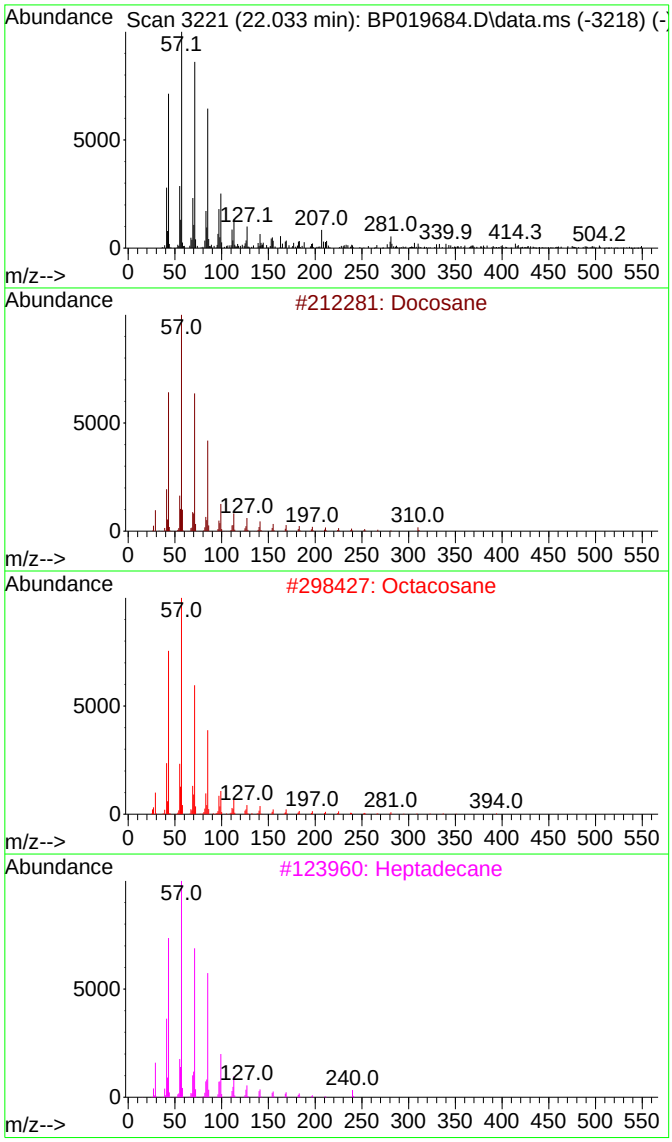
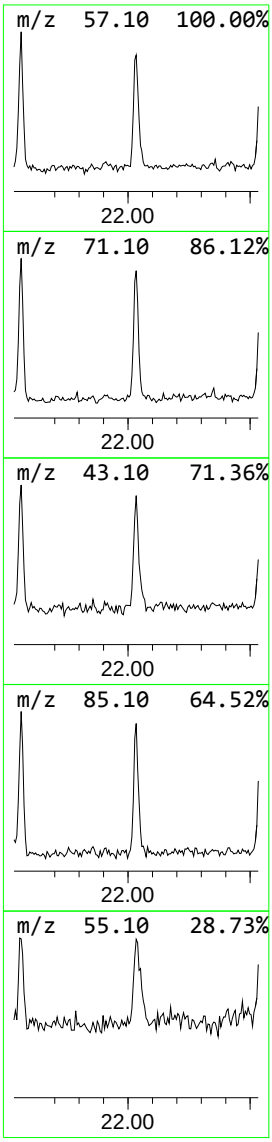
Peak Number 10 Docosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.033	2.07 ng	132567	Chrysene-d12	21.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Heptadecane	240	C17H36	000629-78-7	87
4	Heneicosane	296	C21H44	000629-94-7	83
5	6,6-Diethylhoctadecane	310	C22H46	1000360-41-8	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021324\
Data File : BP019684.D
Acq On : 13 Feb 2024 18:50
Operator : MA/JU
Sample : P1453-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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	3.628	2.8	ng	64225	1	7.905	458386	20.0
2-Pentanone, 4-...	5.022	6.3	ng	144475	1	7.905	458386	20.0
n-Hexadecanoic ...	18.192	10.9	ng	580967	4	17.292	1062140	20.0
Octadecanoic acid	19.427	3.6	ng	231931	5	21.386	1281810	20.0
9-Octadecenamid...	20.545	4.4	ng	280210	5	21.386	1281810	20.0
Adipic acid, 2-...	20.616	4.5	ng	290517	5	21.386	1281810	20.0
Cyclohexadecane	21.110	6.6	ng	424207	5	21.386	1281810	20.0
Tetratriacontan...	21.563	2.0	ng	128973	5	21.386	1281810	20.0
Docosane	22.033	2.1	ng	132567	5	21.386	1281810	20.0