LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008420.D
Acq On : 15 Dec 2021 16:56
Operator : CG/JU
Sample : M5029-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PSC-124019

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-BP121421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008420.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.875	316	321	331	rVB	186463	267242	10.07%	1.708%
2	5.340	395	400	422	rVB	840035	1316431	49.58%	8.416%
3	5.946	498	503	511	rBV	17029	27936	1.05%	0.179%
4	6.940	665	672	698	rBV	704380	1338351	50.41%	8.556%
5	7.740	801	808	817	rBV	189160	301527	11.36%	1.928%
6	8.905	997	1006	1024	rBV	461524	862636	32.49%	5.515%
7	10.540	1276	1284	1295	rBV	204022	391864	14.76%	2.505%
8	13.010	1697	1704	1722	rBV	1083093	1680352	63.29%	10.742%
9	14.393	1934	1939	1948	rVB	313537	480610	18.10%	3.072%
10	15.898	2185	2195	2213	rBV	891816	1472194	55.45%	9.411%
11	17.157	2403	2409	2415	rBV	404429	605536	22.81%	3.871%
12	18.063	2558	2563	2570	rBV2	111922	175433	6.61%	1.122%
13	19.181	2747	2753	2760	rBV	45930	91694	3.45%	0.586%
14	19.304	2771	2774	2783	rBV7	21796	34990	1.32%	0.224%
15	19.534	2811	2813	2825	rVB2	25360	48314	1.82%	0.309%
16	19.728	2841	2846	2854	rBV	2172815	2655039	100.00%	16.973%
17	20.516	2977	2980	2985	rVB	49833	51391	1.94%	0.329%
18	20.822	3028	3032	3036	rBV2	71031	103528	3.90%	0.662%
19	20.975	3054	3058	3068	rVB	314237	432333	16.28%	2.764%
20	21.263	3102	3107	3112	rBV	641008	812837	30.61%	5.196%
21	21.380	3122	3127	3138	rBV	817274	1262437	47.55%	8.071%
22	21.863	3206	3209	3211	rBV	86641	96326	3.63%	0.616%
23	22.351	3289	3292	3298	rVB2	81799	107063	4.03%	0.684%
24	22.898	3381	3385	3389	rBV2	102415	171383	6.46%	1.096%
25	23.627	3504	3509	3518	rVB2	447079	855081	32.21%	5.466%

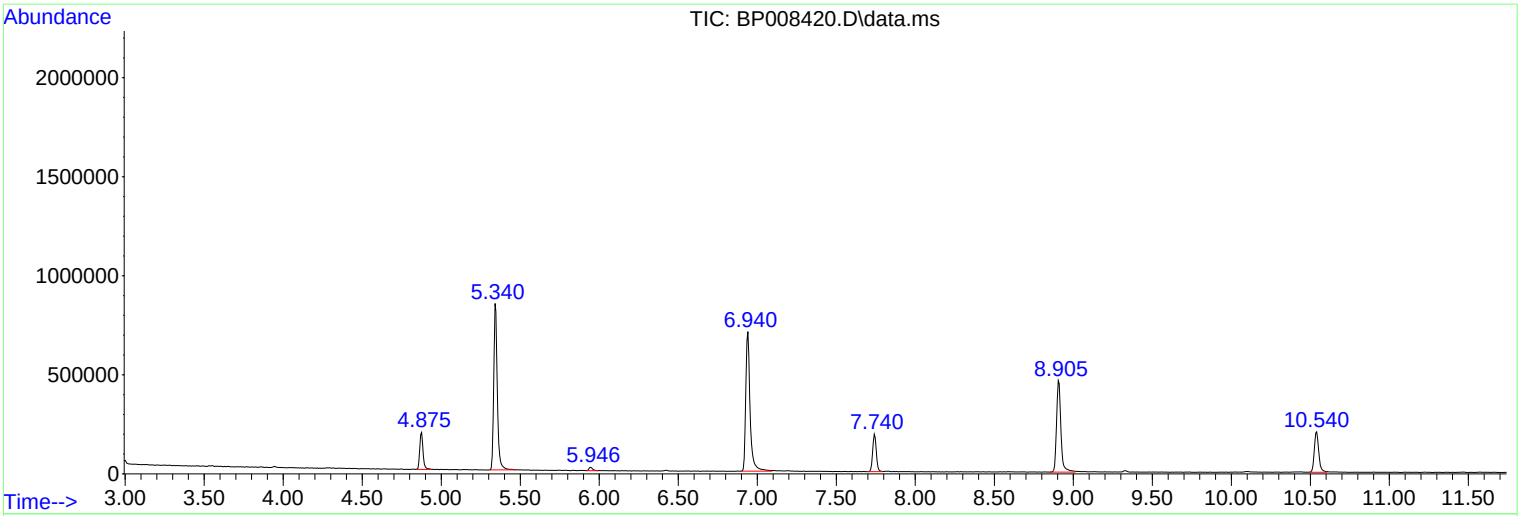
Sum of corrected areas: 15642528

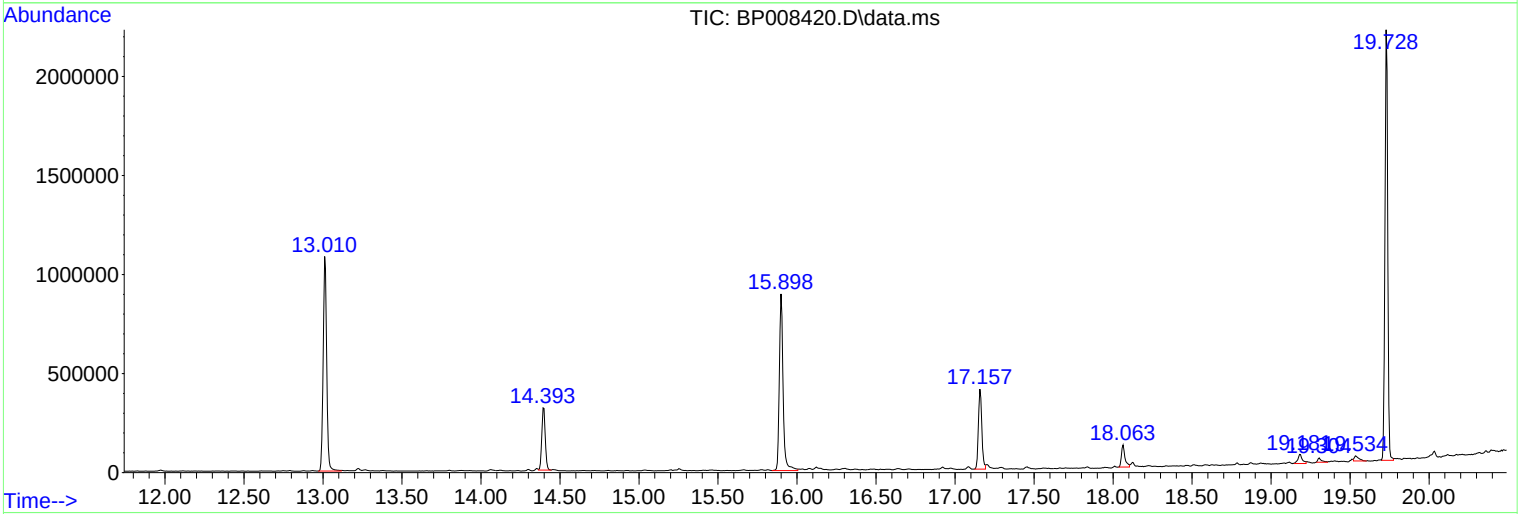
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008420.D
Acq On : 15 Dec 2021 16:56
Operator : CG/JU
Sample : M5029-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

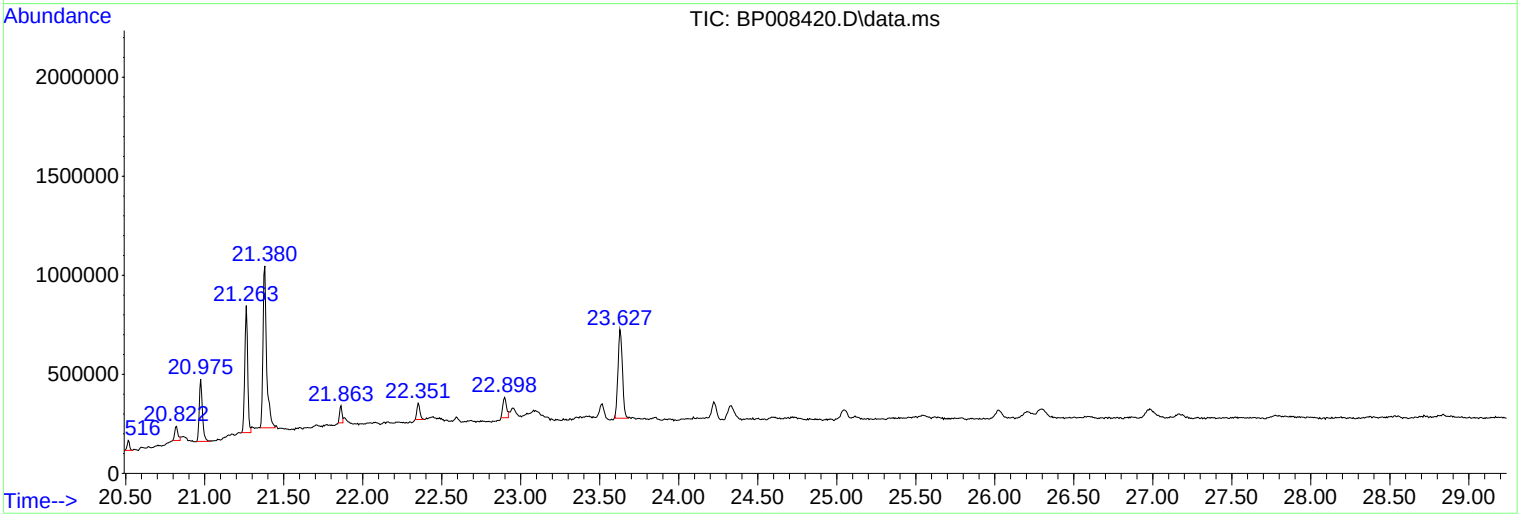
Instrument :
BNA_P
ClientSampleId :
PSC-124019

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.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\BP121521\
Data File : BP008420.D
Acq On : 15 Dec 2021 16:56
Operator : CG/JU
Sample : M5029-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PSC-124019

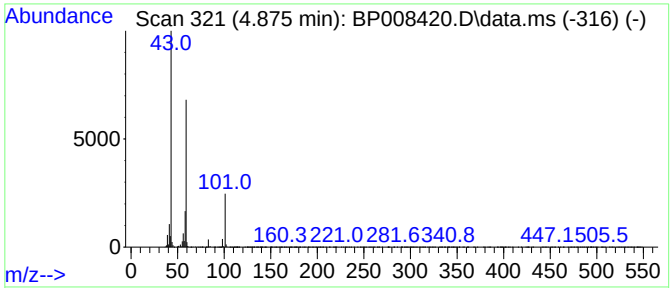
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

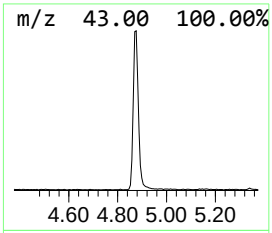
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

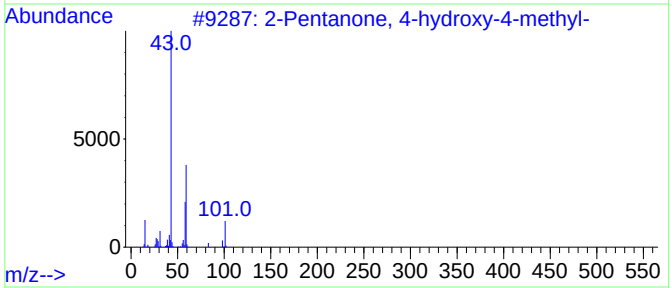
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

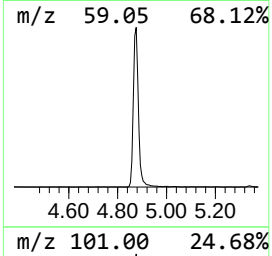
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.875	17.73 ng	267242	1,4-Dichlorobenzene-d4	7.740

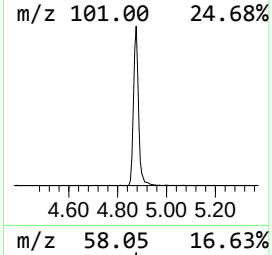
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Acetone	58	C3H6O	000067-64-1	10

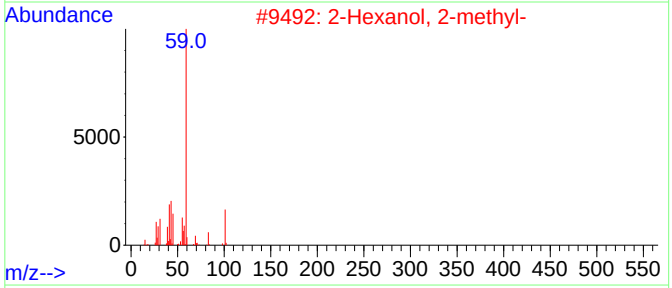


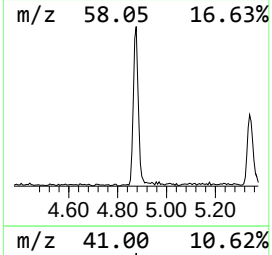


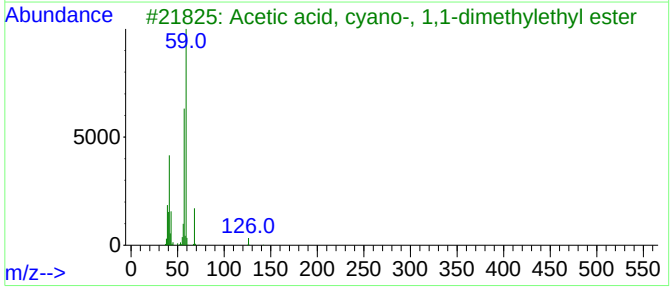


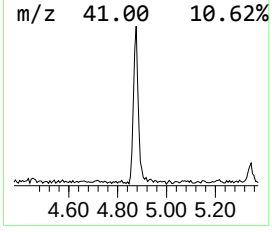












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008420.D
Acq On : 15 Dec 2021 16:56
Operator : CG/JU
Sample : M5029-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PSC-124019

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

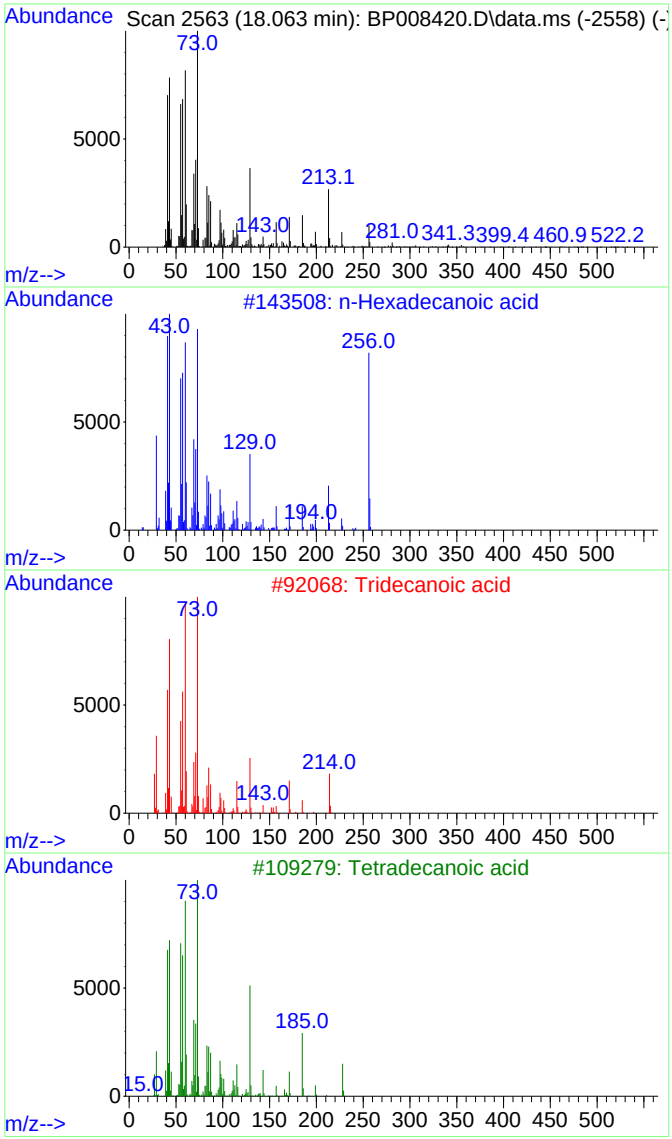
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

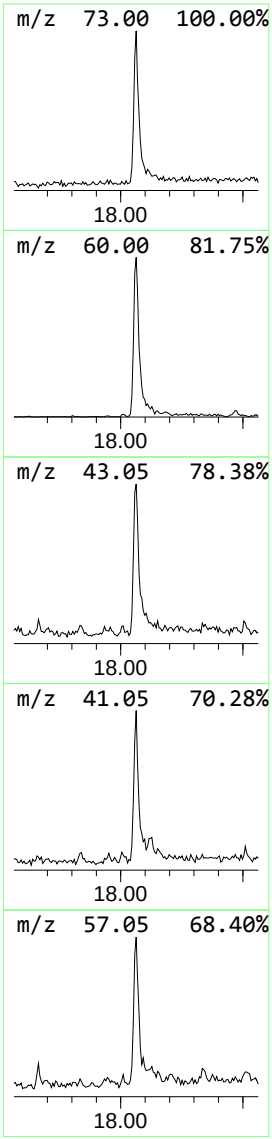
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.063	5.79 ng	175433	Phenanthrene-d10	17.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Octadecanoic acid	284	C18H36O2	000057-11-4	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008420.D
Acq On : 15 Dec 2021 16:56
Operator : CG/JU
Sample : M5029-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PSC-124019

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

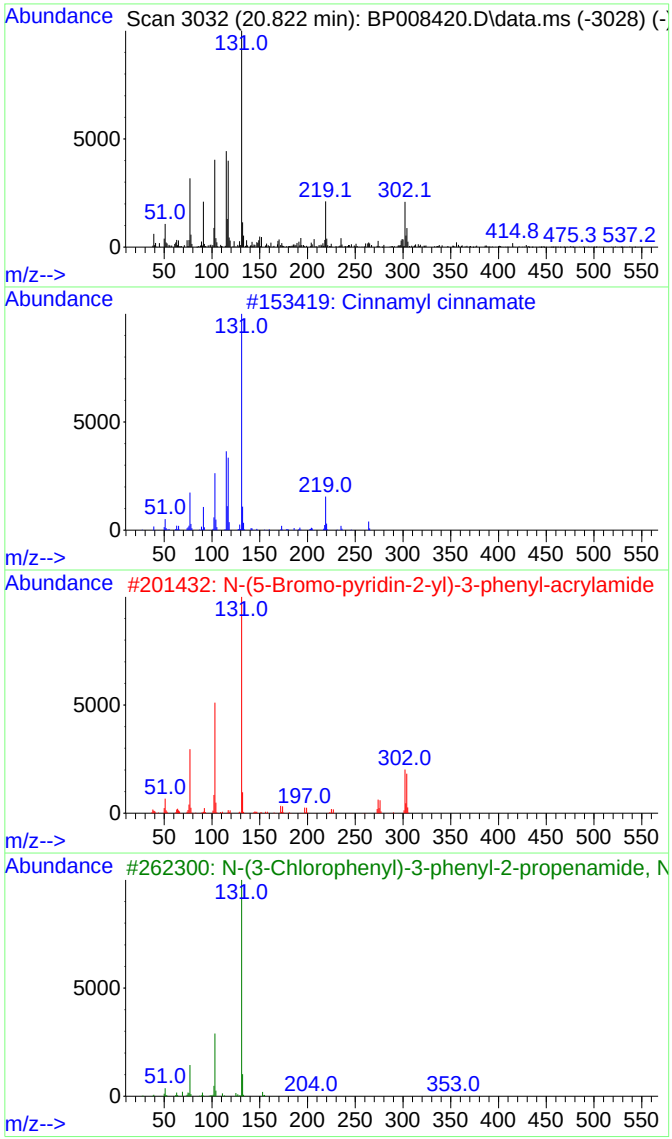
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

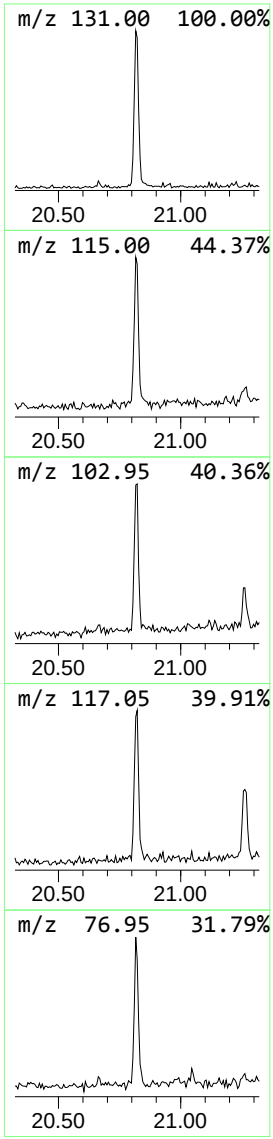
****

Peak Number 4 Cinnamyl cinnamate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.822	2.55 ng	103528	Chrysene-d12	21.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	80
2	N-(5-Bromo-pyridin-2-yl)-3-pheny...	302	C14H11BrN2O	328119-25-1	70
3	N-(3-Chlorophenyl)-3-phenyl-2-pr...	353	C17H11ClF3NO2	1000492-37-1	46
4	N-(2-Chlorophenyl)-3-phenyl-2-pr...	353	C17H11ClF3NO2	1000492-36-9	41
5	Vinyl trans-cinnamate	174	C11H10O2	017719-70-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008420.D
Acq On : 15 Dec 2021 16:56
Operator : CG/JU
Sample : M5029-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PSC-124019

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

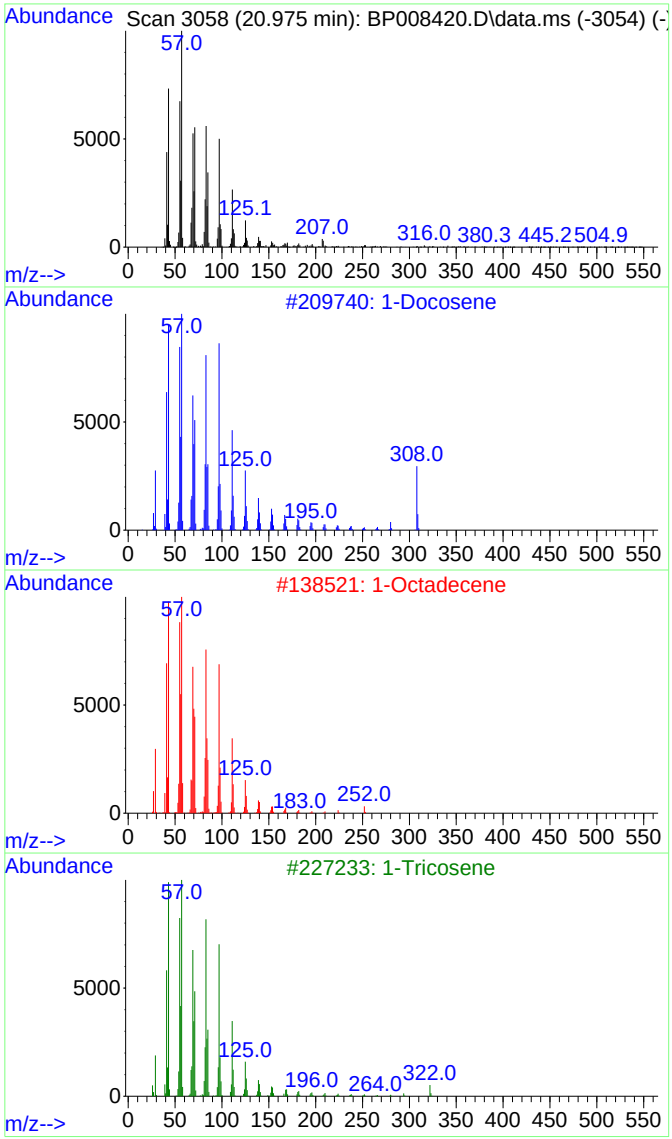
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

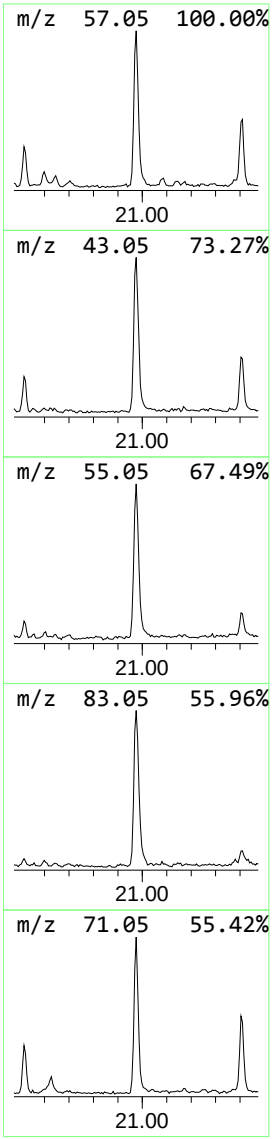
****

Peak Number 5 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.975	10.64 ng	432333	Chrysene-d12	21.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	97
2	1-Octadecene	252	C18H36	000112-88-9	97
3	1-Tricosene	322	C23H46	018835-32-0	95
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	95
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008420.D
Acq On : 15 Dec 2021 16:56
Operator : CG/JU
Sample : M5029-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PSC-124019

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

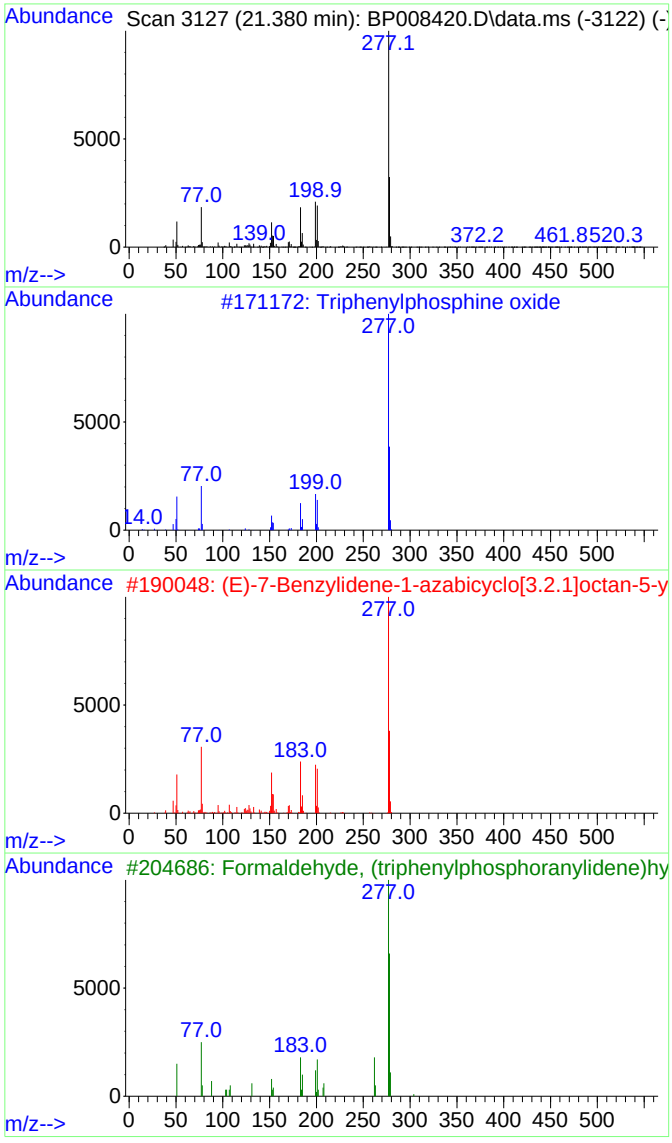
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

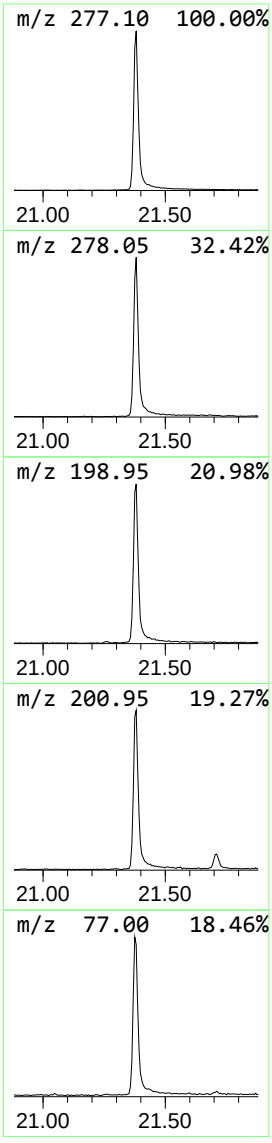
****

Peak Number 6 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.381	31.06 ng	1262440	Chrysene-d12	21.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	90
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4	3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	37
5	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008420.D
Acq On : 15 Dec 2021 16:56
Operator : CG/JU
Sample : M5029-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PSC-124019

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

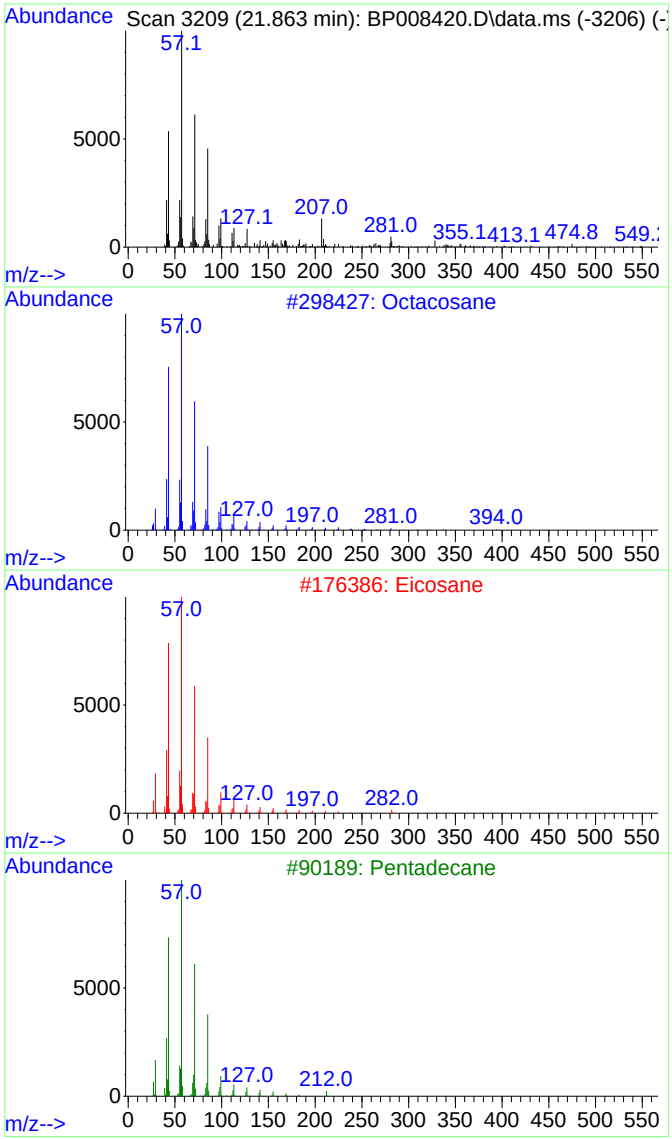
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

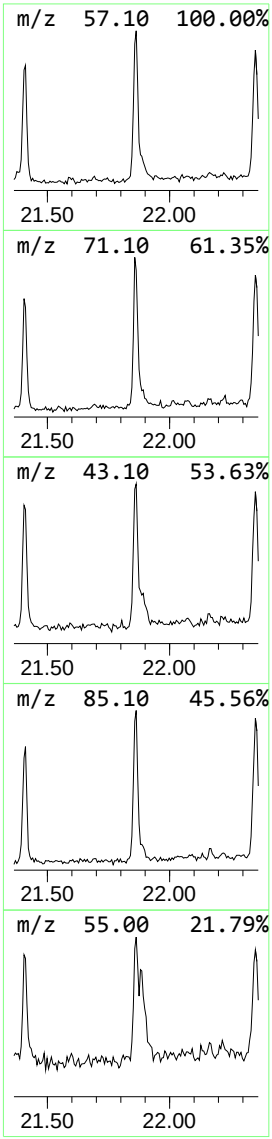
****

Peak Number 7 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.863	2.37 ng	96326	Chrysene-d12	21.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	97
2	Eicosane	282	C20H42	000112-95-8	90
3	Pentadecane	212	C15H32	000629-62-9	89
4	Hexacosane	366	C26H54	000630-01-3	87
5	Tricosane, 2-methyl-	338	C24H50	001928-30-9	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008420.D
Acq On : 15 Dec 2021 16:56
Operator : CG/JU
Sample : M5029-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PSC-124019

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

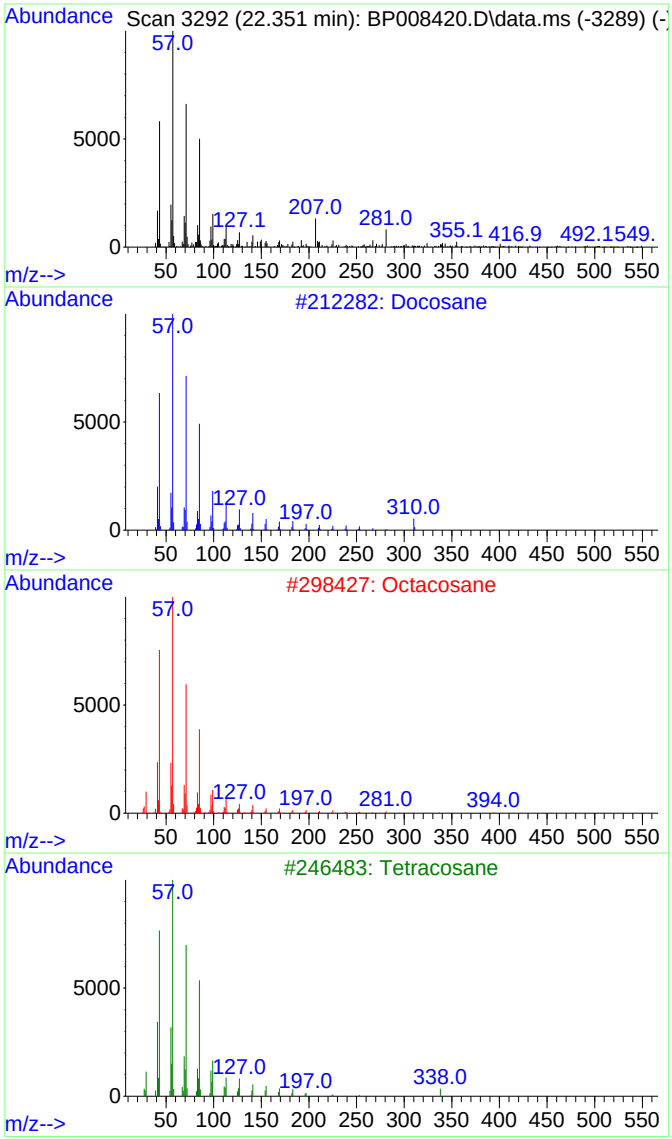
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

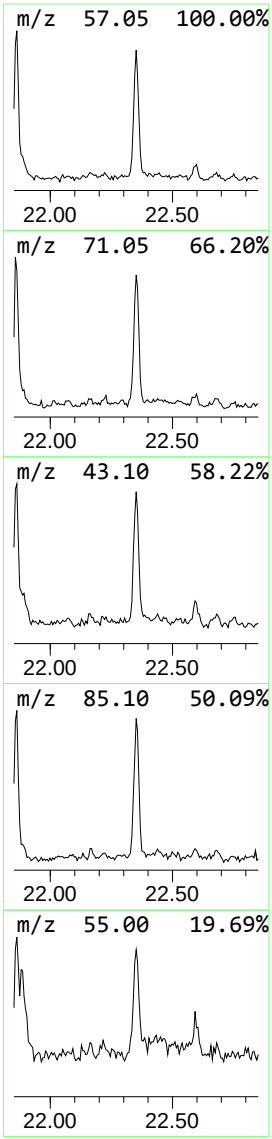
****

Peak Number 8 Docosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.351	2.63 ng	107063	Chrysene-d12	21.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	97
2	Octacosane	394	C28H58	000630-02-4	96
3	Tetracosane	338	C24H50	000646-31-1	93
4	Tricosane	324	C23H48	000638-67-5	89
5	Heptadecane	240	C17H36	000629-78-7	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008420.D
Acq On : 15 Dec 2021 16:56
Operator : CG/JU
Sample : M5029-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PSC-124019

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

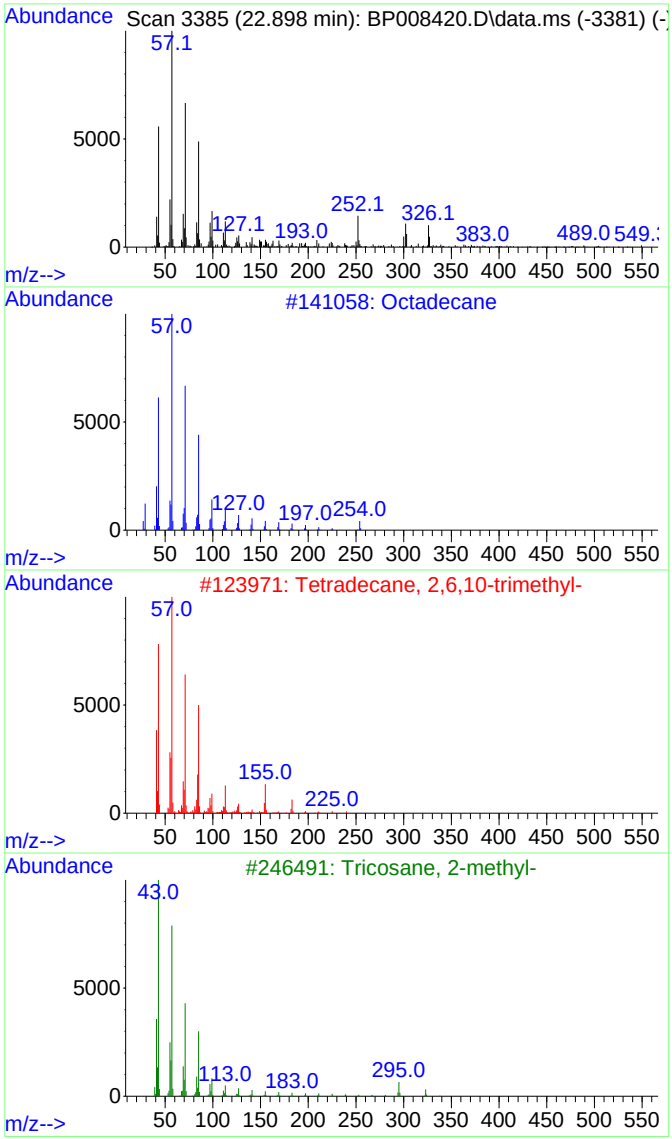
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

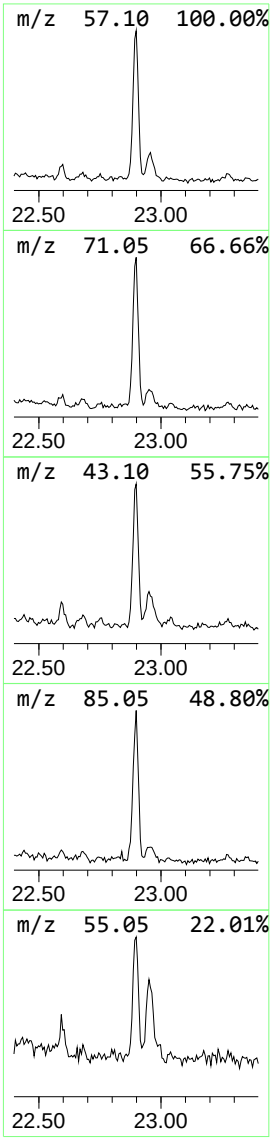
****

Peak Number 9 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.898	4.01 ng	171383	Perylene-d12	23.627

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	90
2	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	78
3	Tricosane, 2-methyl-	338	C24H50	001928-30-9	78
4	Pentacosane	352	C25H52	000629-99-2	60
5	Octacosane	394	C28H58	000630-02-4	60





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008420.D
Acq On : 15 Dec 2021 16:56
Operator : CG/JU
Sample : M5029-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PSC-124019

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.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
2-Pentanone, 4-...	4.875	17.7	ng	267242	1	7.740	301527	20.0
n-Hexadecanoic ...	18.063	5.8	ng	175433	4	17.157	605536	20.0
Cinnamyl cinnamate	20.822	2.5	ng	103528	5	21.263	812837	20.0
1-Docosene	20.975	10.6	ng	432333	5	21.263	812837	20.0
Triphenylphosph...	21.381	31.1	ng	1262440	5	21.263	812837	20.0
Octacosane	21.863	2.4	ng	96326	5	21.263	812837	20.0
Docosane	22.351	2.6	ng	107063	5	21.263	812837	20.0
Octadecane	22.898	4.0	ng	171383	6	23.627	855081	20.0