LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019835.D
Acq On : 22 Feb 2024 21:12
Operator : MA/JU
Sample : P1521-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CG-MW-17-CH3

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: BP019835.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.893	284	307	312	rVV	173862	738557	1.80%	1.024%
2	5.016	316	328	345	rVB2	182292	437949	1.07%	0.607%
3	5.475	399	406	412	rBV	725951	1342302	3.27%	1.861%
4	7.069	670	677	693	rVB2	465835	954567	2.33%	1.323%
5	7.893	810	817	825	rBV	278329	456090	1.11%	0.632%
6	8.728	941	959	963	rBV	14216348	41017200	100.00%	56.862%
7	9.075	1011	1018	1026	rBV	844583	1529293	3.73%	2.120%
8	9.263	1035	1050	1055	rBV	289461	875059	2.13%	1.213%
9	10.134	1191	1198	1207	rBV	1517787	2471392	6.03%	3.426%
10	10.693	1286	1293	1298	rBV	354630	628525	1.53%	0.871%
11	11.298	1386	1396	1403	rBV	279350	657108	1.60%	0.911%
12	12.575	1595	1613	1623	rBV	860156	2416498	5.89%	3.350%
13	13.157	1705	1712	1721	rBV	2476951	3716514	9.06%	5.152%
14	14.528	1939	1945	1953	rBV2	580019	979494	2.39%	1.358%
15	16.028	2193	2200	2210	rBV	2083047	3188814	7.77%	4.421%
16	17.286	2406	2414	2421	rBV	741183	1162781	2.83%	1.612%
17	18.192	2562	2568	2576	rBV	755768	1056188	2.57%	1.464%
18	19.316	2755	2759	2770	rVV2	199463	538593	1.31%	0.747%
19	19.422	2773	2777	2785	rVB3	305326	424572	1.04%	0.589%
20	19.857	2846	2851	2861	rVV	4158722	5119858	12.48%	7.098%
21	21.386	3106	3111	3118	rBV	913624	1218456	2.97%	1.689%
22	23.810	3517	3523	3532	rVB	573929	1204719	2.94%	1.670%

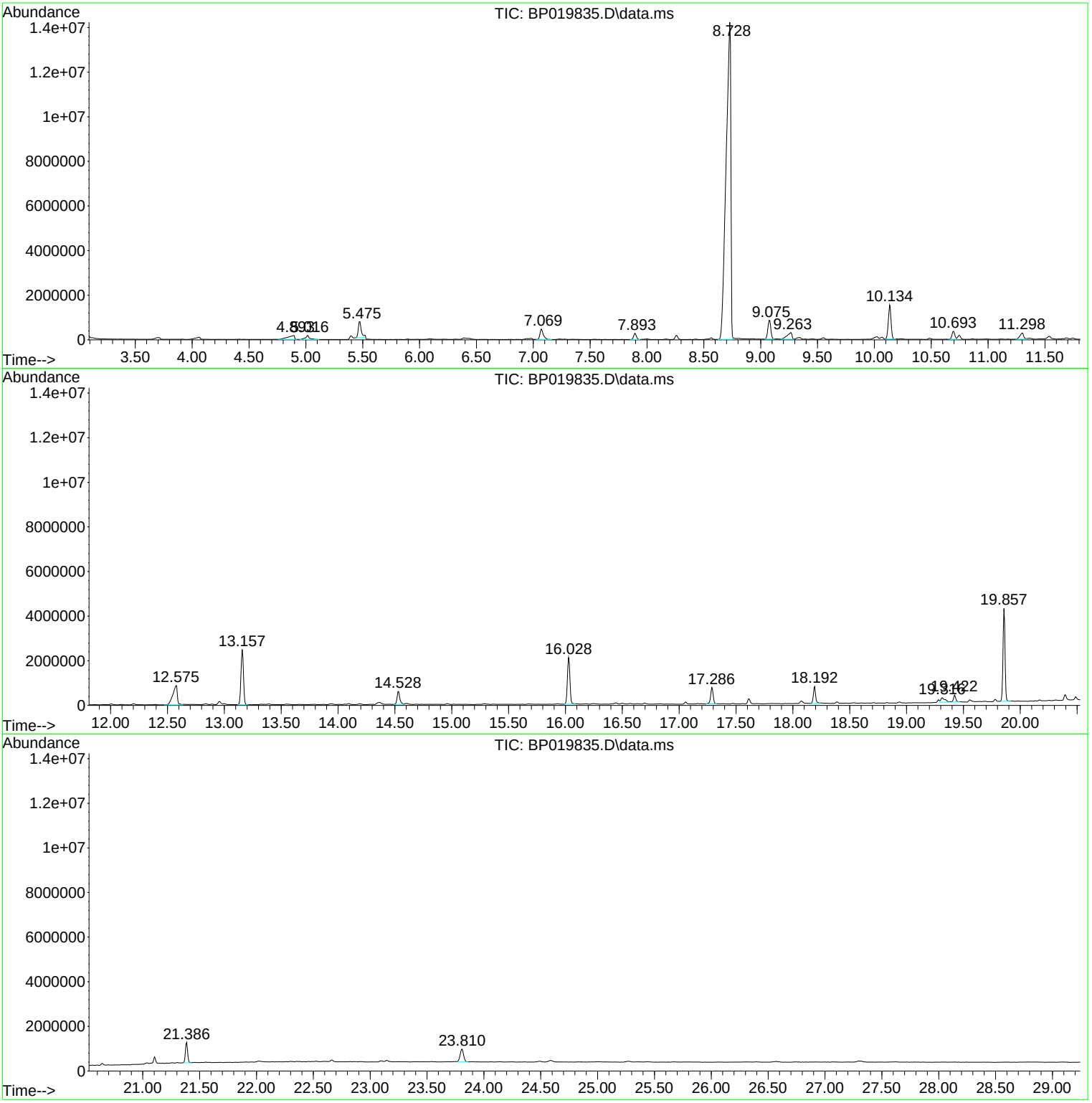
Sum of corrected areas: 72134529

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019835.D
Acq On : 22 Feb 2024 21:12
Operator : MA/JU
Sample : P1521-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-17-CH3

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\BP022224\
Data File : BP019835.D
Acq On : 22 Feb 2024 21:12
Operator : MA/JU
Sample : P1521-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-17-CH3

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

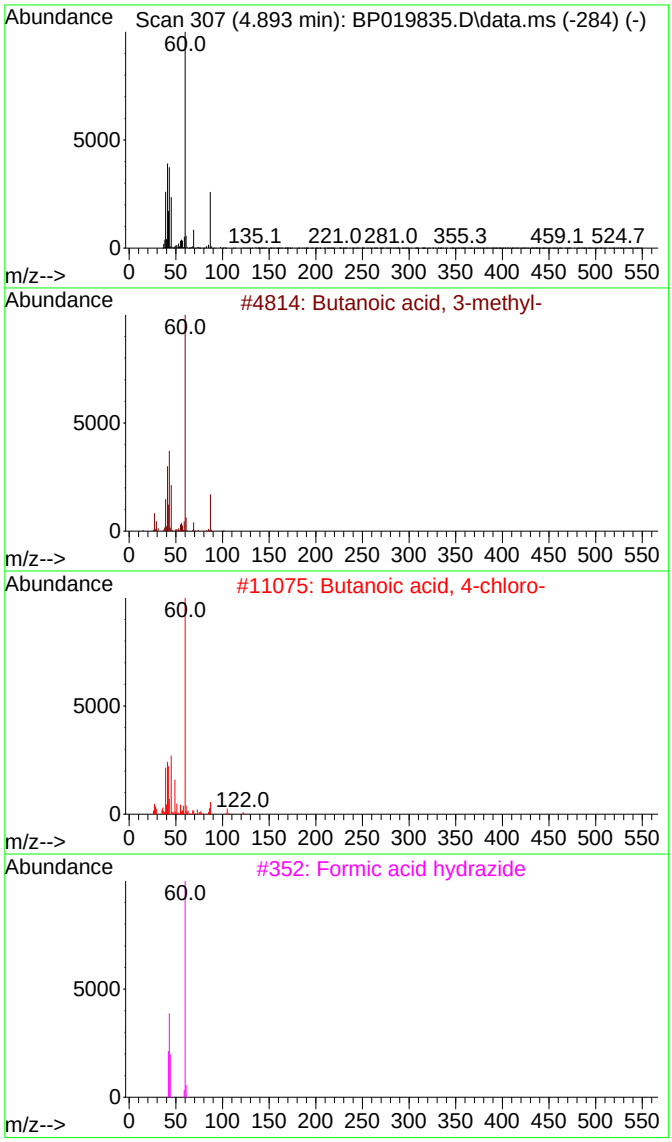
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

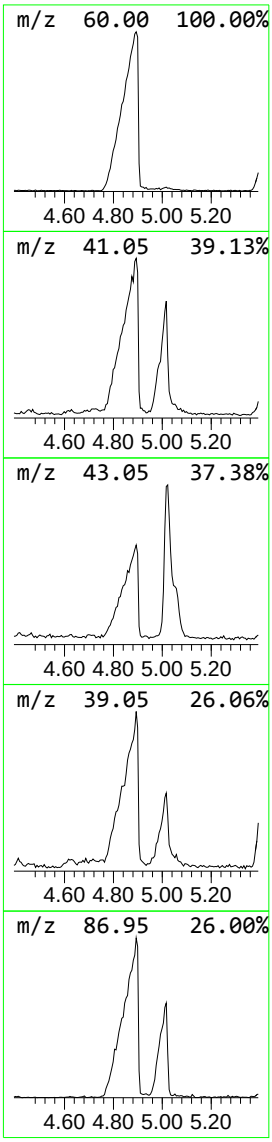
****

Peak Number 1 Butanoic acid, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.893	32.39 ng	738557	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	78
2	Butanoic acid, 4-chloro-	122	C4H7ClO2	000627-00-9	50
3	Formic acid hydrazide	60	CH4N2O	000624-84-0	47
4	1-Hexanamine	101	C6H15N	000111-26-2	9
5	Pentanoic acid	102	C5H10O2	000109-52-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019835.D
Acq On : 22 Feb 2024 21:12
Operator : MA/JU
Sample : P1521-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-17-CH3

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

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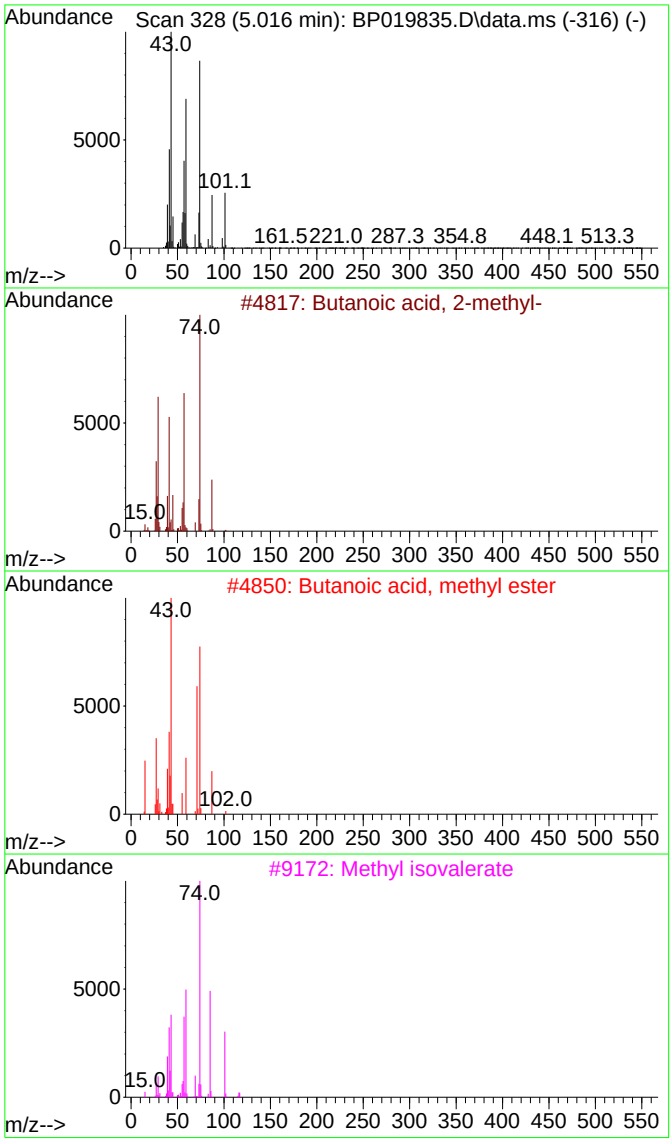
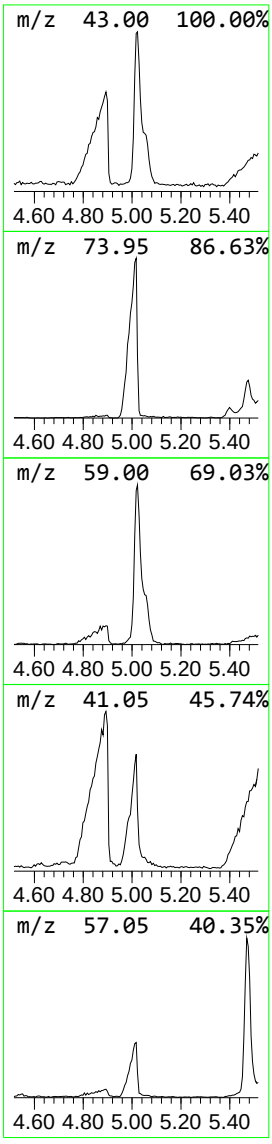
Peak Number 2 Butanoic acid, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	19.20 ng	437949	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	47
2	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	43
3	Methyl isovalerate	116	C6H12O2	000556-24-1	38
4	Dodecanoic acid, 2-methyl-	214	C13H26O2	002874-74-0	32
5	3-Heptanol, 5-methyl-	130	C8H18O	018720-65-5	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019835.D
Acq On : 22 Feb 2024 21:12
Operator : MA/JU
Sample : P1521-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-17-CH3

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

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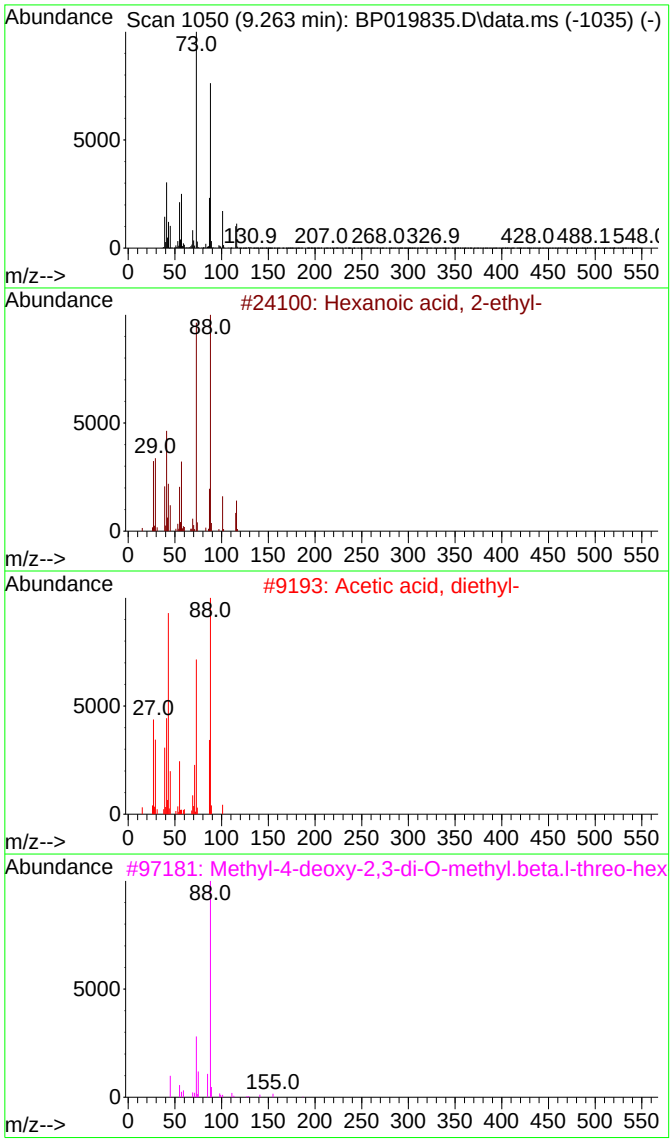
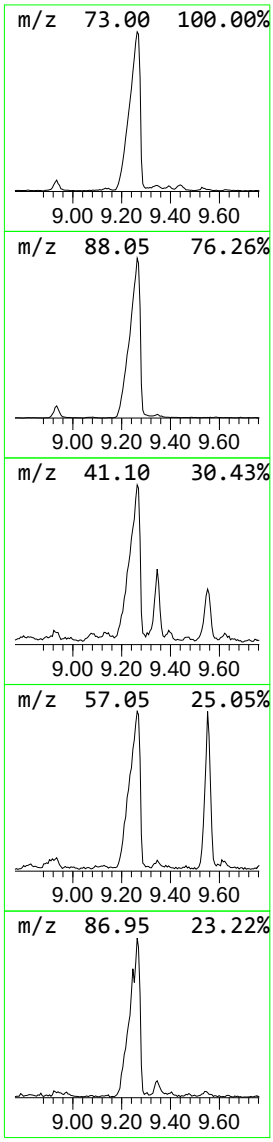
Peak Number 3 Hexanoic acid, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.263	38.37 ng	875059	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	50
3	Methyl-4-deoxy-2,3-di-O-methyl.b...	218	C9H14O6	1000312-09-9	47
4	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	45
5	Butyl mannoside, tetramethyl ether	292	C14H28O6	1000501-84-1	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019835.D
Acq On : 22 Feb 2024 21:12
Operator : MA/JU
Sample : P1521-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-17-CH3

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

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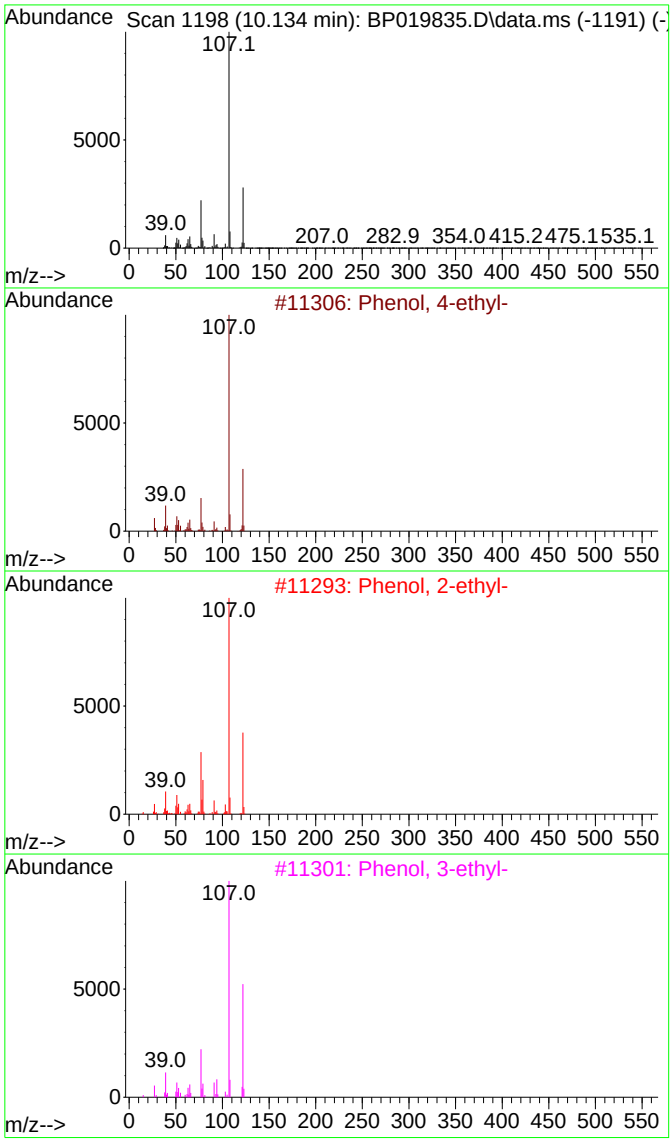
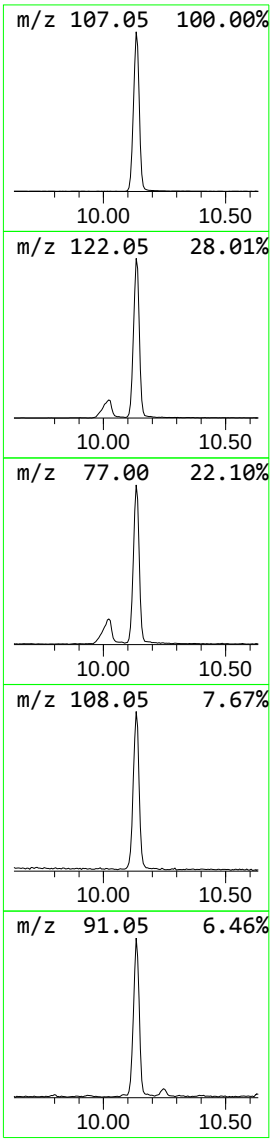
Peak Number 4 Phenol, 4-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.134	78.64 ng	2471390	Naphthalene-d8	10.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-ethyl-	122	C8H10O	000123-07-9	93
2	Phenol, 2-ethyl-	122	C8H10O	000090-00-6	91
3	Phenol, 3-ethyl-	122	C8H10O	000620-17-7	91
4	Phenol, 3,4-dimethyl-	122	C8H10O	000095-65-8	78
5	Phenol, 2,5-dimethyl-	122	C8H10O	000095-87-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019835.D
Acq On : 22 Feb 2024 21:12
Operator : MA/JU
Sample : P1521-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-17-CH3

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

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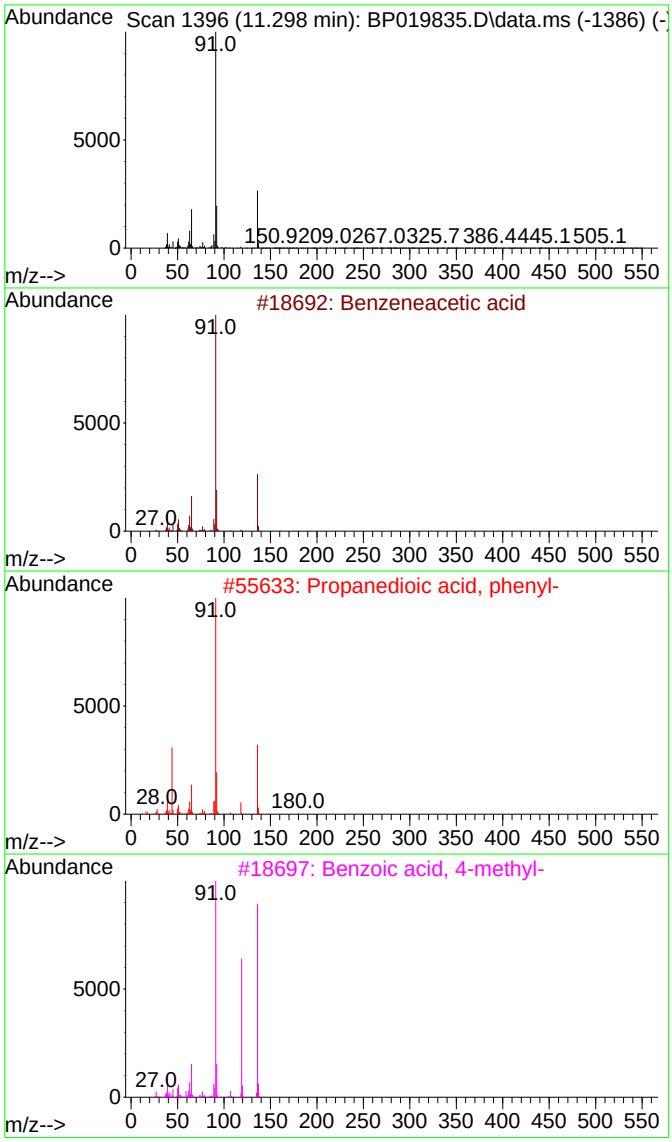
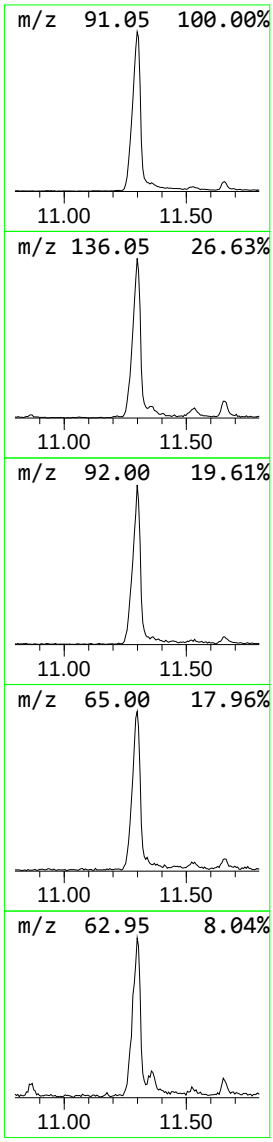
Peak Number 5 Benzeneacetic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.298	20.91 ng	657108	Naphthalene-d8	10.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetic acid	136	C8H8O2	000103-82-2	95
2	Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	83
3	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	59
4	3-Oxo-4-phenylbutyronitrile	159	C10H9NO	019212-27-2	53
5	Benzeneacetaldehyde	120	C8H8O	000122-78-1	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019835.D
Acq On : 22 Feb 2024 21:12
Operator : MA/JU
Sample : P1521-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-17-CH3

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

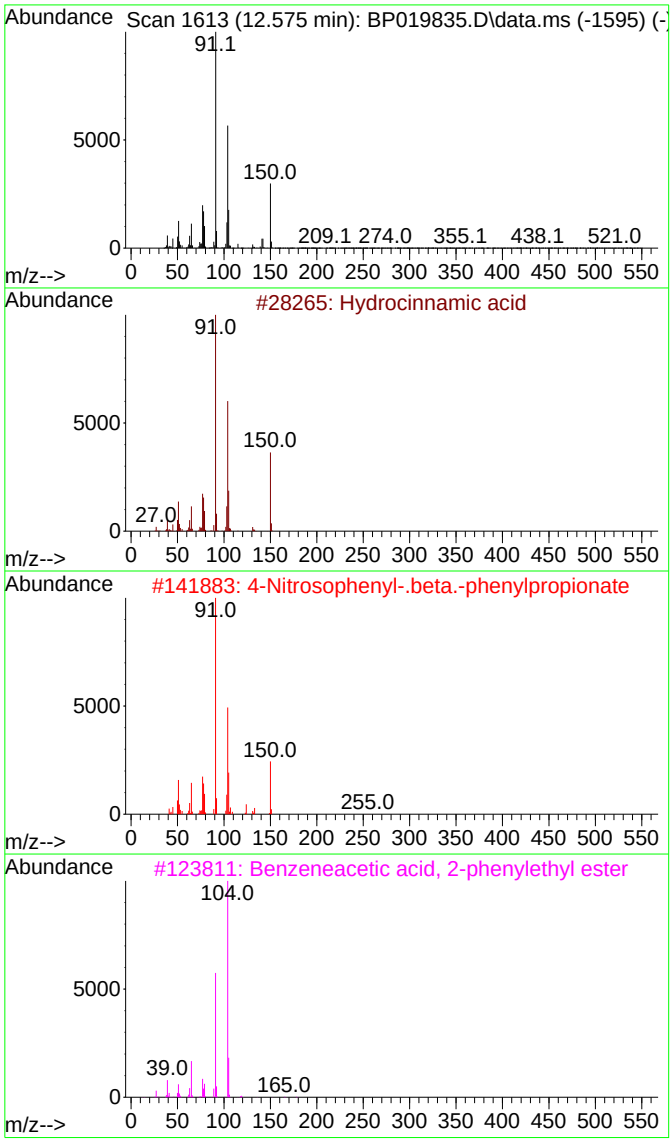
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

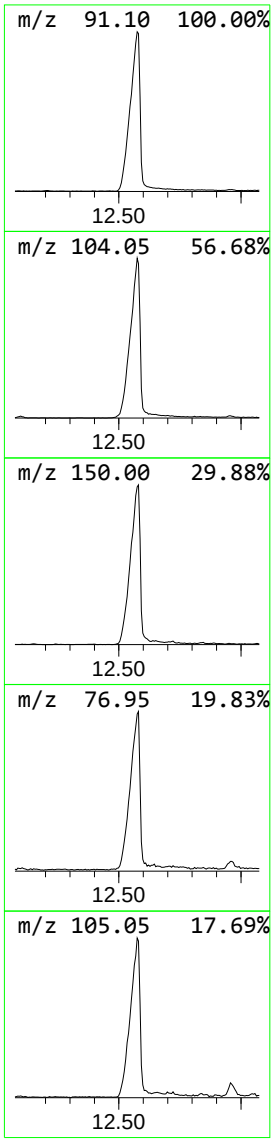
****

Peak Number 6 Hydrocinnamic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.575	76.89 ng	2416500	Naphthalene-d8	10.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrocinnamic acid	150	C9H10O2	000501-52-0	96
2	4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	86
3	Benzeneacetic acid, 2-phenylethy...	240	C16H16O2	000102-20-5	47
4	Acetic acid, trifluoro-, 2-pheny...	218	C10H9F3O2	055419-66-4	46
5	Benzene, (2-nitroethyl)-	151	C8H9NO2	006125-24-2	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019835.D
Acq On : 22 Feb 2024 21:12
Operator : MA/JU
Sample : P1521-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-17-CH3

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

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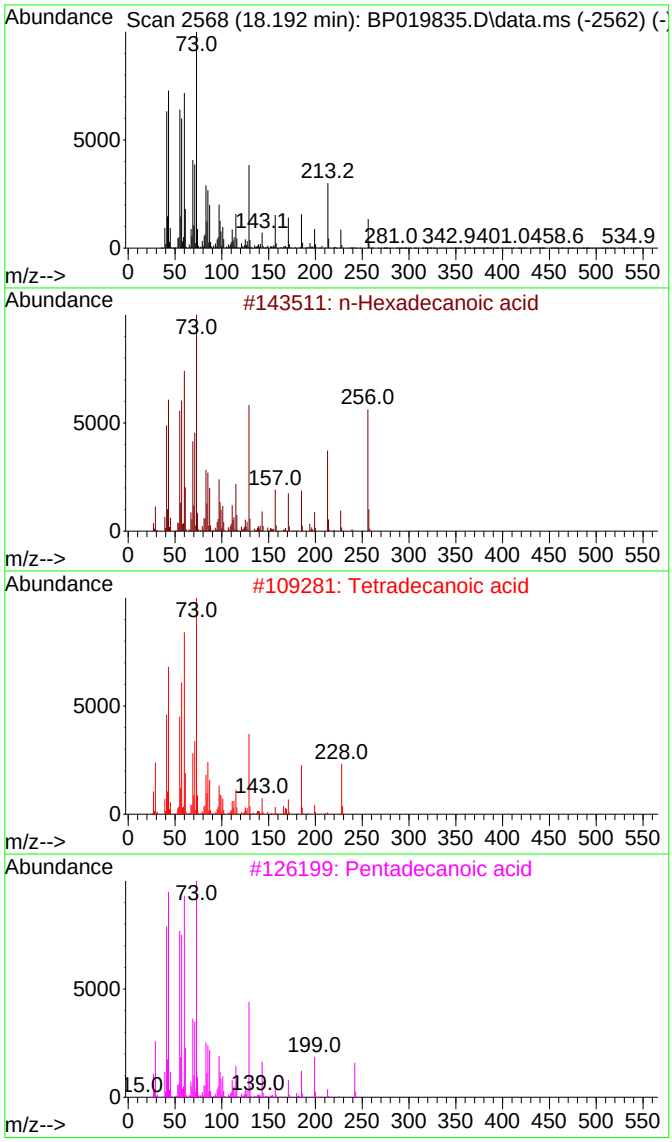
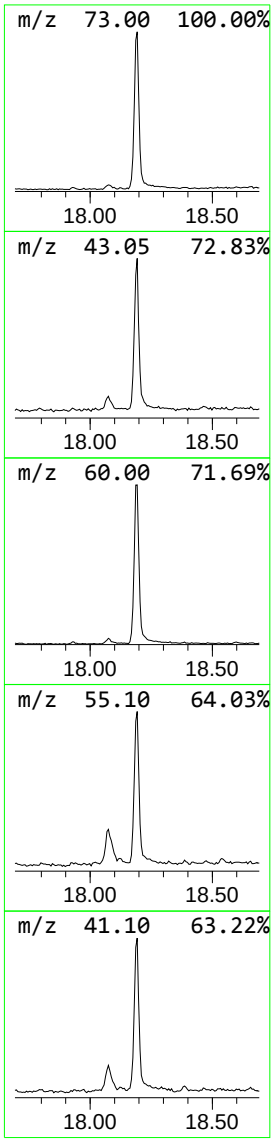
Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	18.17 ng	1056190	Phenanthrene-d10	17.286

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	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	86
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019835.D
Acq On : 22 Feb 2024 21:12
Operator : MA/JU
Sample : P1521-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-17-CH3

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

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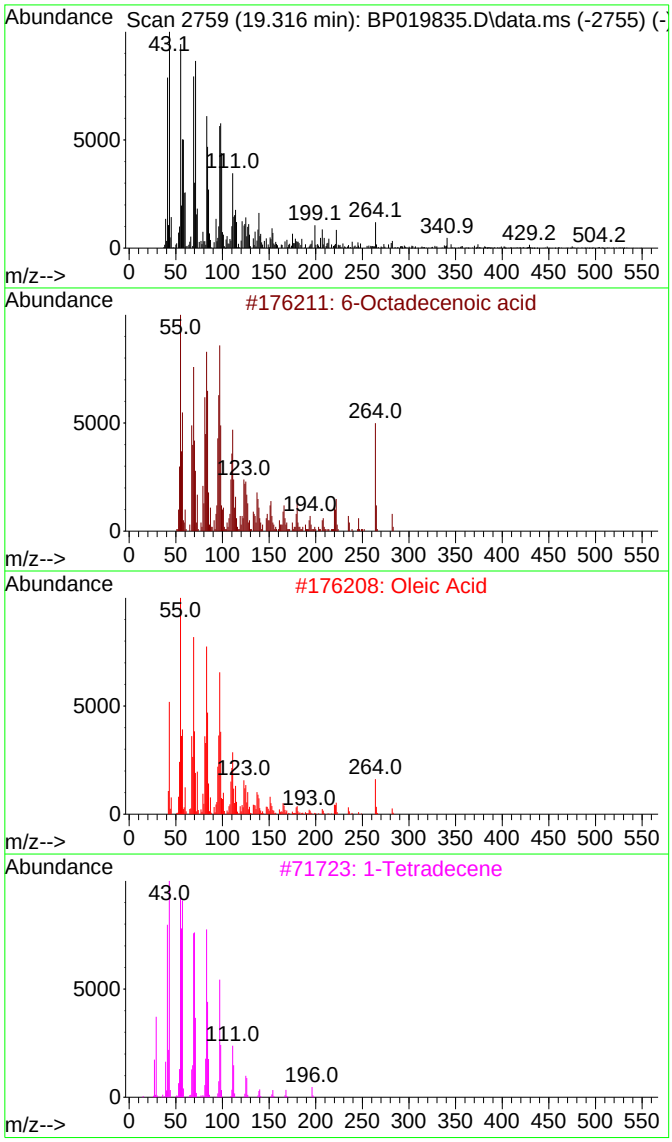
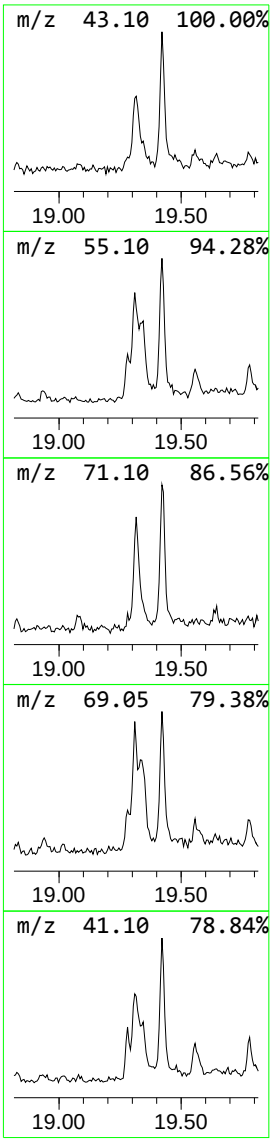
Peak Number 8 6-Octadecenoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.316	9.26 ng	538593	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid	282	C18H34O2	1000336-66-8	70
2	Oleic Acid	282	C18H34O2	000112-80-1	70
3	1-Tetradecene	196	C14H28	001120-36-1	55
4	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	50
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	46





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Data File : BP019835.D
Acq On : 22 Feb 2024 21:12
Operator : MA/JU
Sample : P1521-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-17-CH3

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

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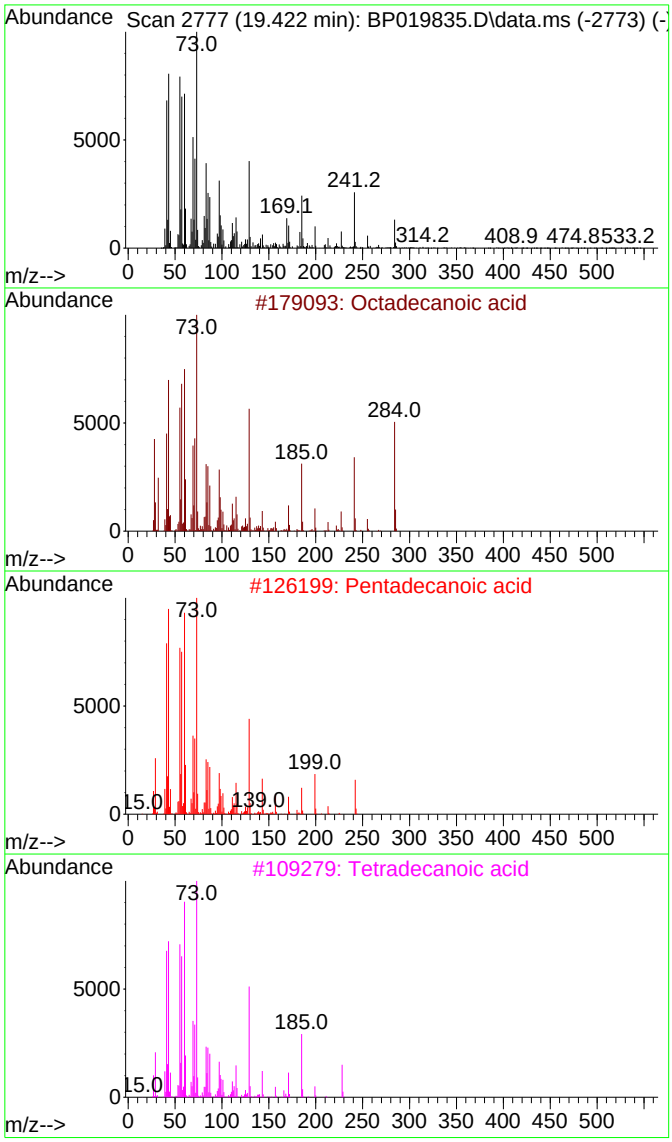
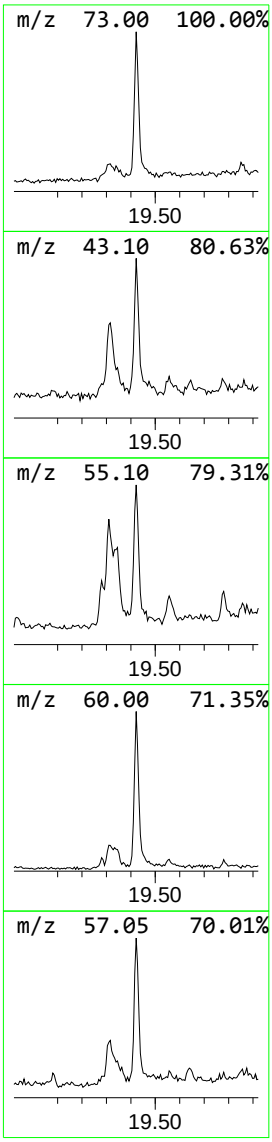
Peak Number 9 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.422	6.97 ng	424572	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	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	53
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019835.D
Acq On : 22 Feb 2024 21:12
Operator : MA/JU
Sample : P1521-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-17-CH3

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
Butanoic acid, ...	4.893	32.4	ng	738557	1	7.893	456090	20.0
Butanoic acid, ...	5.016	19.2	ng	437949	1	7.893	456090	20.0
Hexanoic acid, ...	9.263	38.4	ng	875059	1	7.893	456090	20.0
Phenol, 4-ethyl-	10.134	78.6	ng	2471390	2	10.693	628525	20.0
Benzeneacetic acid	11.298	20.9	ng	657108	2	10.693	628525	20.0
Hydrocinnamic acid	12.575	76.9	ng	2416500	2	10.693	628525	20.0
n-Hexadecanoic ...	18.192	18.2	ng	1056190	4	17.286	1162780	20.0
6-Octadecenoic ...	19.316	9.3	ng	538593	4	17.286	1162780	20.0
Octadecanoic acid	19.422	7.0	ng	424572	5	21.386	1218460	20.0