LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061324\
Data File : BP020616.D
Acq On : 13 Jun 2024 18:06
Operator : MA/JU
Sample : P2864-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WC-H

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-BP052924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP020616.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.023	3	6	24	rVB	2064216	2967682	26.17%	4.617%
2	3.552	92	96	108	rVB	228216	321126	2.83%	0.500%
3	4.922	322	329	337	rVB2	227316	353576	3.12%	0.550%
4	5.370	397	405	412	rBV	3547147	5156184	45.47%	8.022%
5	6.928	662	670	686	rBV	3316396	5399959	47.62%	8.401%
6	7.752	800	810	817	rBV	747730	1283183	11.31%	1.996%
7	8.899	997	1005	1014	rBV	2001478	3465906	30.56%	5.392%
8	9.446	1091	1098	1112	rVB	100291	163824	1.44%	0.255%
9	10.299	1236	1243	1253	rBV	135847	296876	2.62%	0.462%
10	10.516	1270	1280	1287	rBV	1046616	1762905	15.54%	2.743%
11	11.257	1393	1406	1417	rBV	166850	345450	3.05%	0.537%
12	12.987	1692	1700	1715	rBV	4889318	8174161	72.08%	12.717%
13	14.375	1927	1936	1944	rBV	1559473	2380541	20.99%	3.704%
14	14.598	1967	1974	1980	rVB3	110027	239628	2.11%	0.373%
15	15.892	2187	2194	2206	rBV	4190748	6716150	59.22%	10.449%
16	17.187	2407	2414	2419	rBV	1863373	2835252	25.00%	4.411%
17	17.492	2462	2466	2474	rVB	141679	208303	1.84%	0.324%
18	18.134	2570	2575	2596	rBV	1102846	1783427	15.73%	2.775%
19	19.328	2772	2778	2783	rBV4	59905	161089	1.42%	0.251%
20	19.457	2796	2800	2813	rBV	521733	875503	7.72%	1.362%
21	19.916	2871	2878	2887	rBV	8154057	11340806	100.00%	17.644%
22	21.327	3113	3118	3128	rBV	649415	1229704	10.84%	1.913%
23	21.645	3166	3172	3178	rBV2	1616138	2929770	25.83%	4.558%
24	23.251	3441	3445	3459	rVB4	378092	948088	8.36%	1.475%
25	24.986	3733	3740	3751	rVB2	1033063	2935839	25.89%	4.568%

Sum of corrected areas: 64274932

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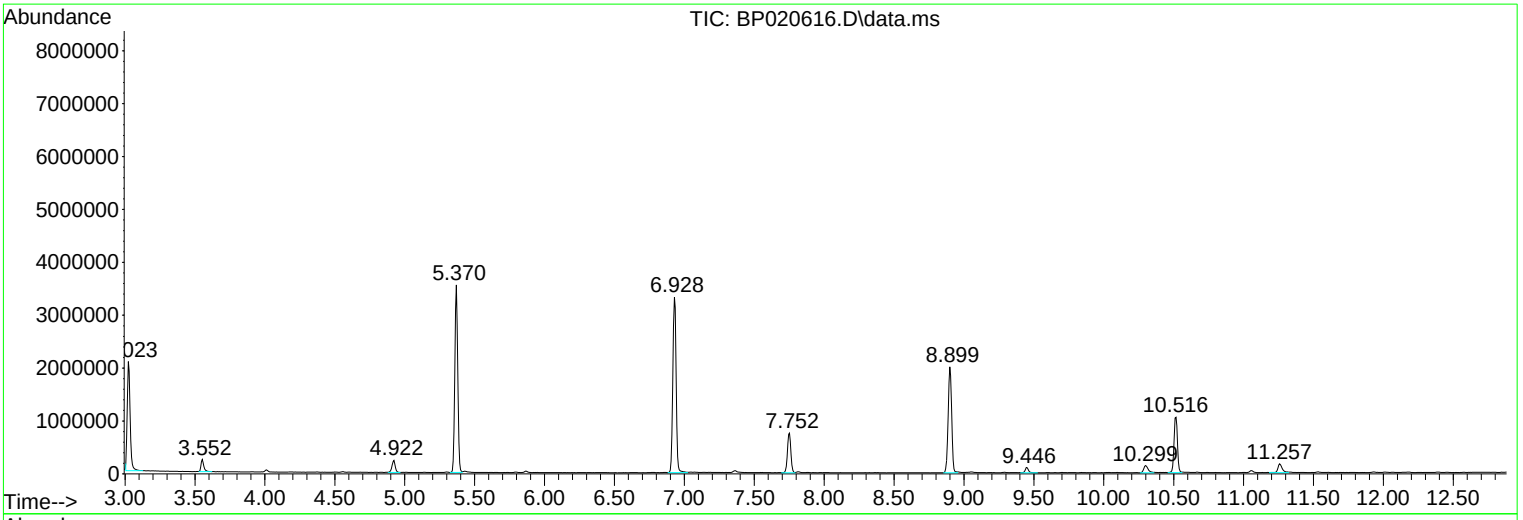
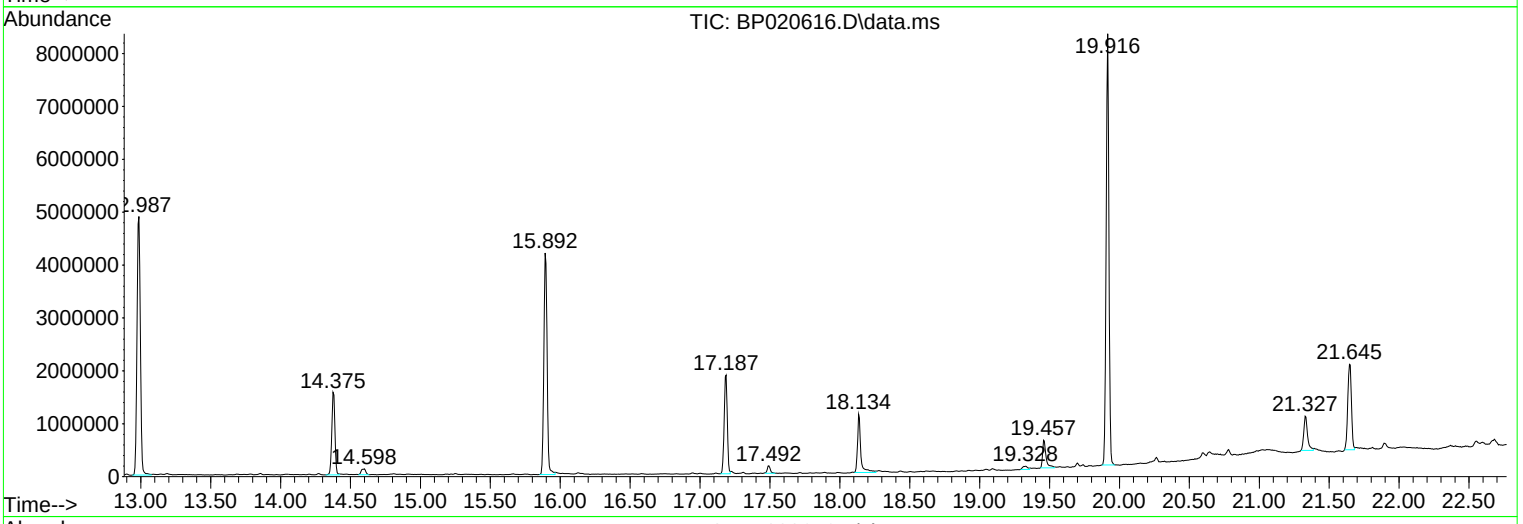
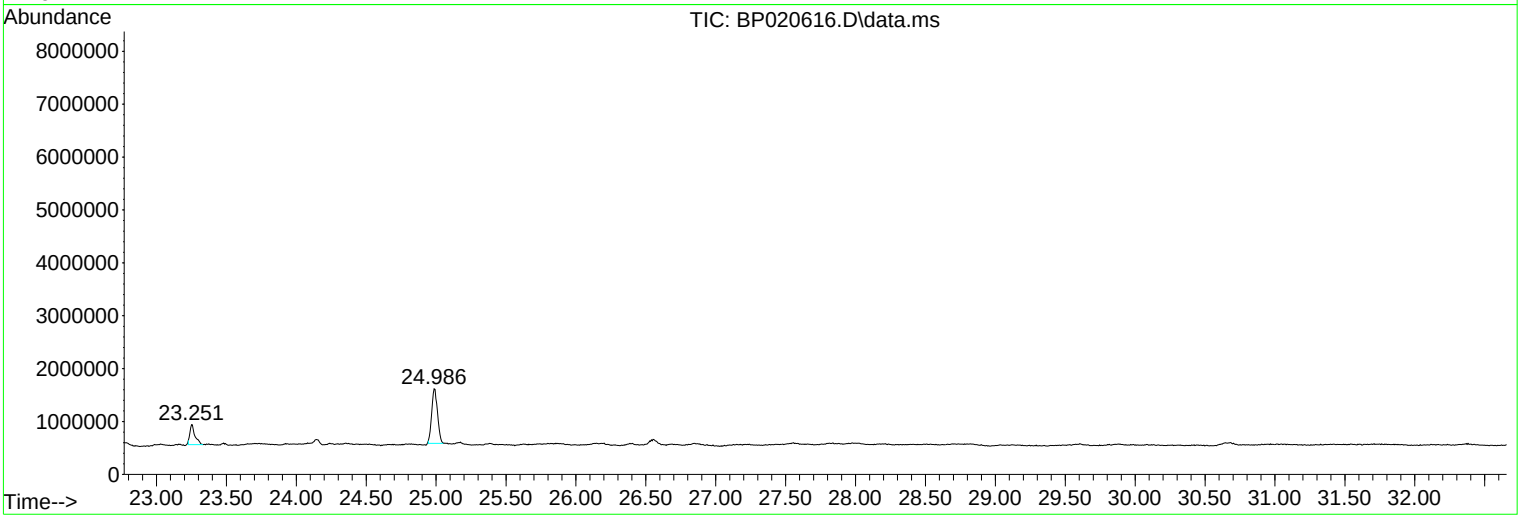
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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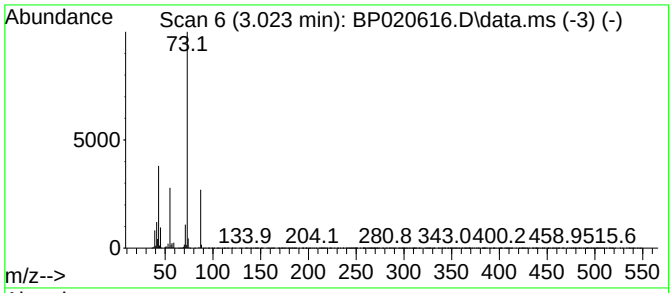
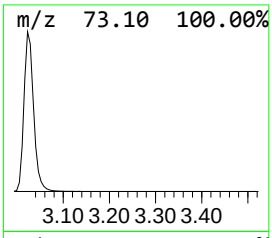
****

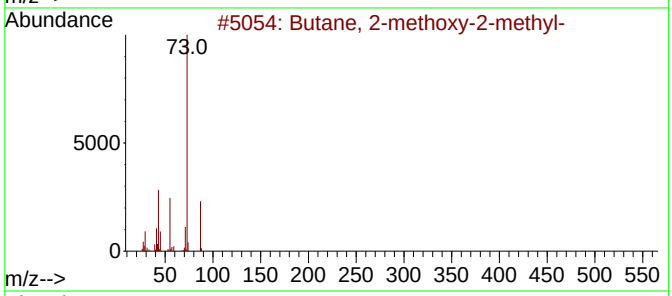
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

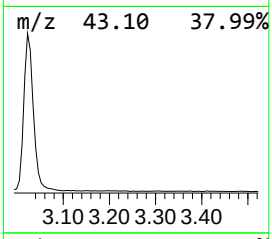
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.023	46.26 ng	2967680	1,4-Dichlorobenzene-d4	7.752

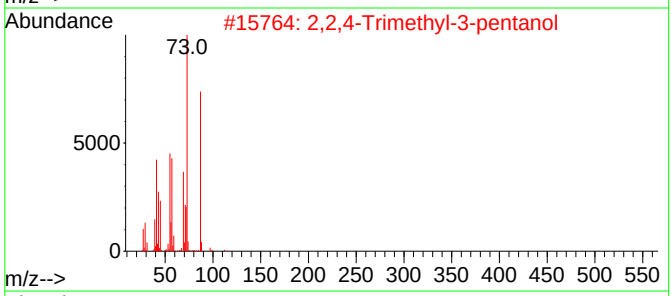
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9

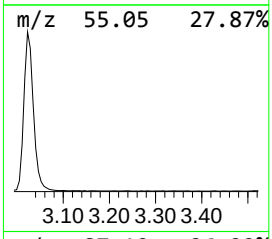


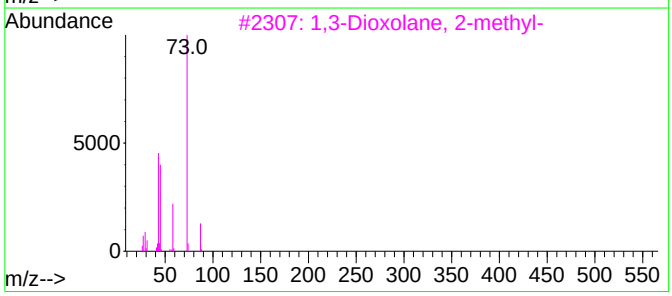


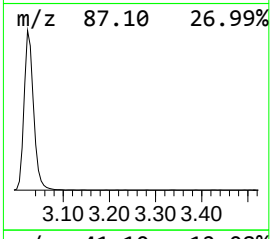


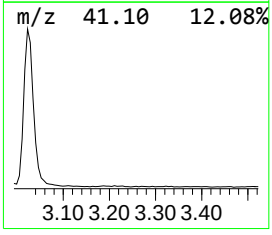












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061324\
Data File : BP020616.D
Acq On : 13 Jun 2024 18:06
Operator : MA/JU
Sample : P2864-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WC-H

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

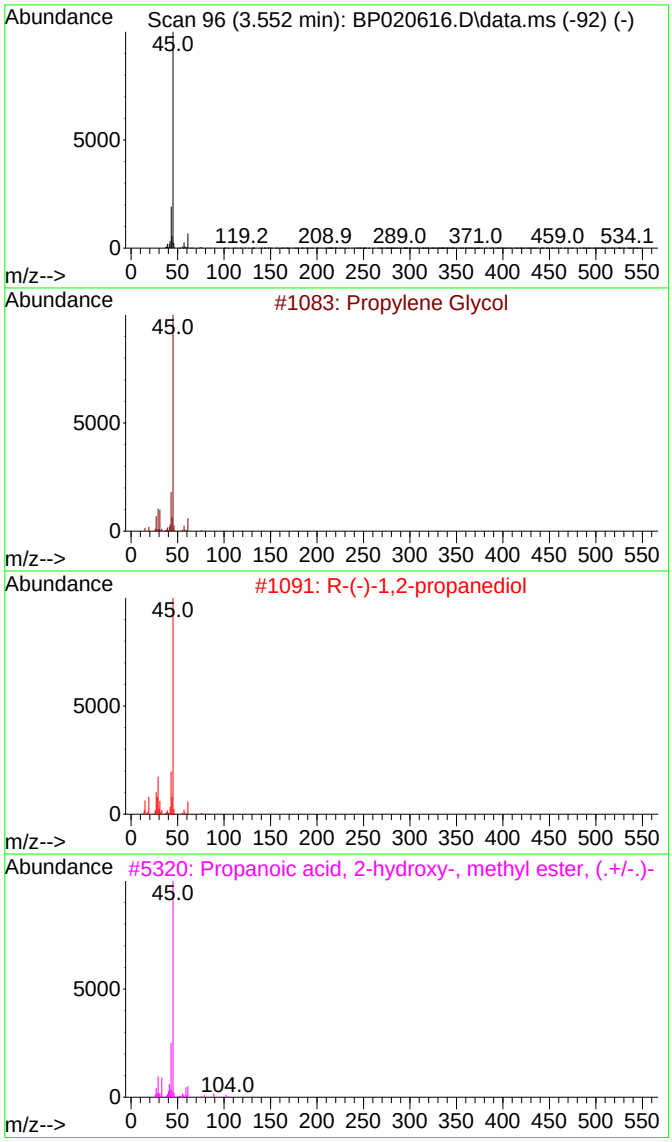
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

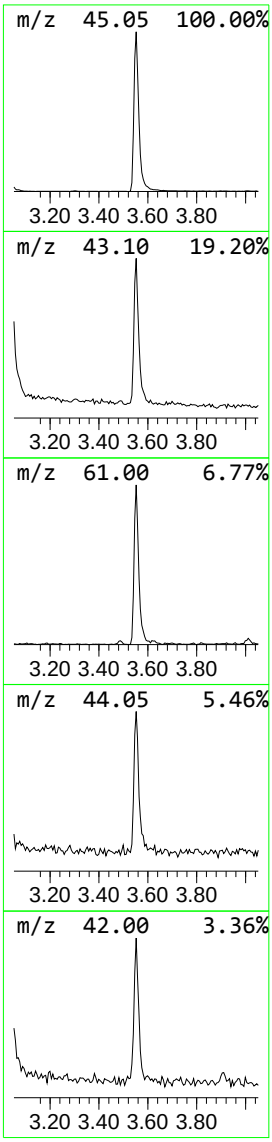
****

Peak Number 2 Propylene Glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.552	5.01 ng	321126	1,4-Dichlorobenzene-d4	7.752

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	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	72
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061324\
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Sample : P2864-01
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ALS Vial : 8 Sample Multiplier: 1

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BNA_P
ClientSampleId :
WC-H

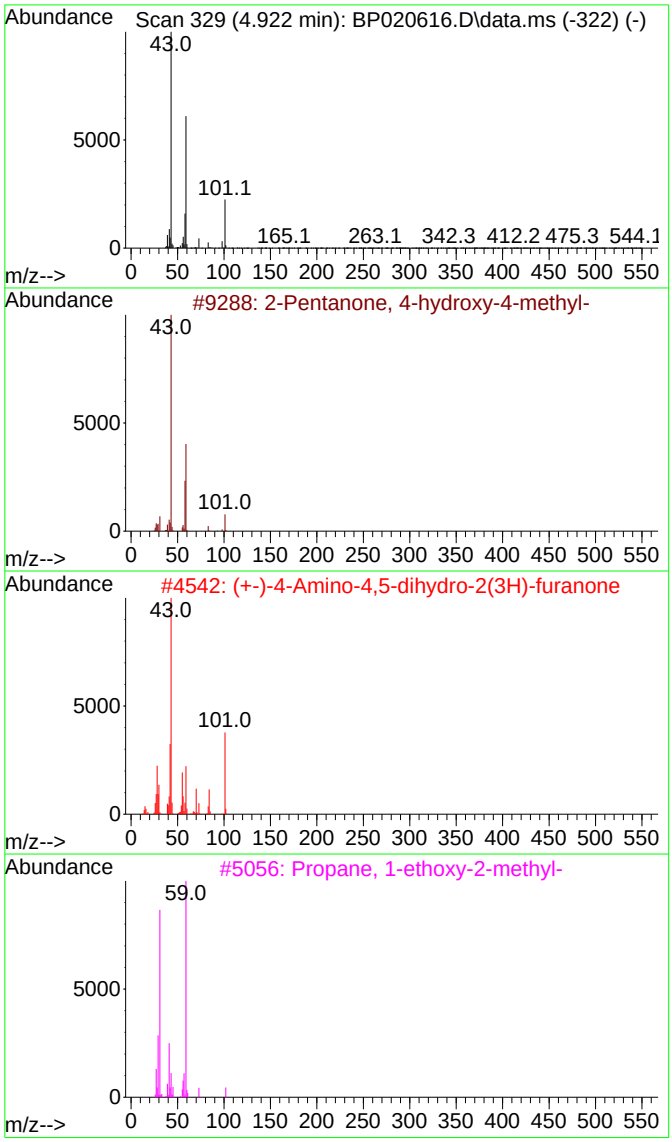
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

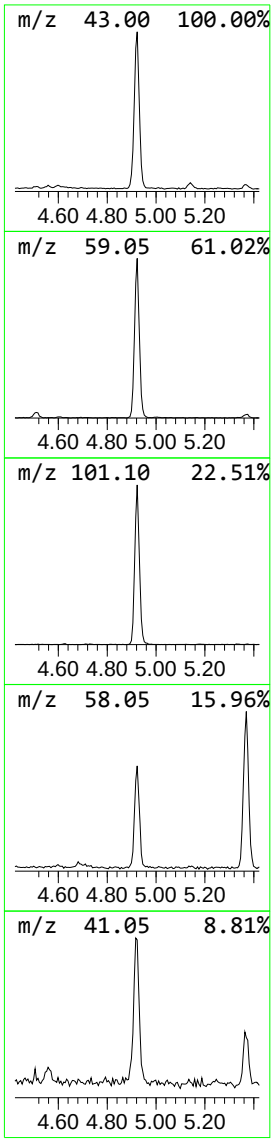
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.922	5.51 ng	353576	1,4-Dichlorobenzene-d4	7.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	32
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	32
4	Hexanamide	115	C6H13NO	000628-02-4	27
5	Methyl 2-(2-(2-methoxyethoxy)eth...	192	C8H16O5	1000366-88-2	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061324\
Data File : BP020616.D
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Operator : MA/JU
Sample : P2864-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

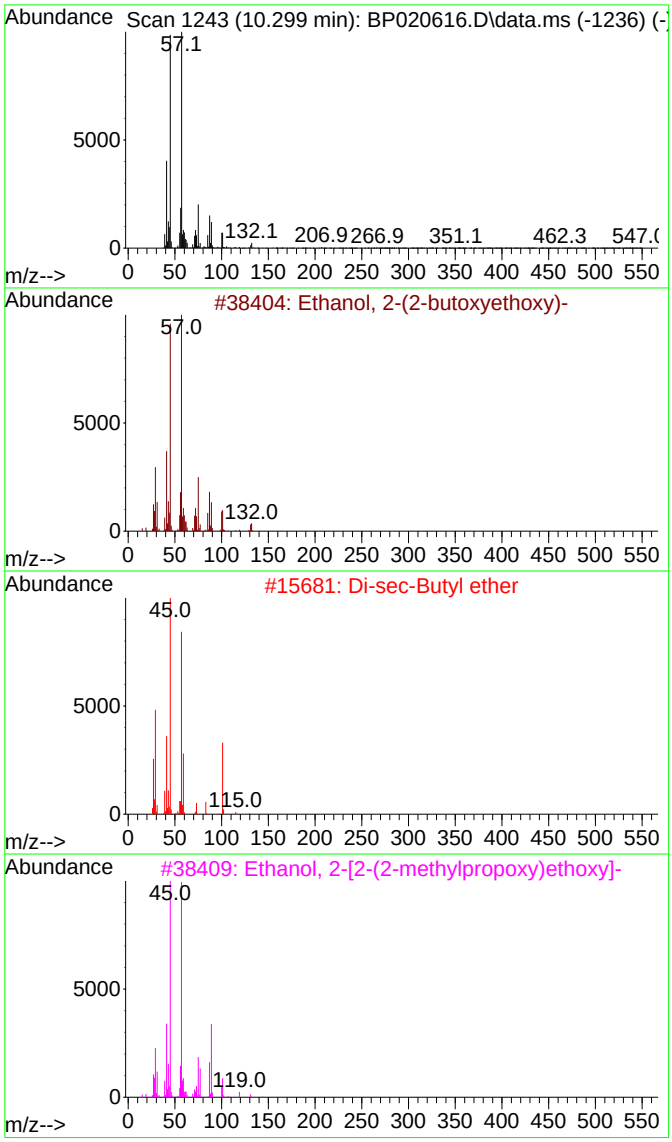
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

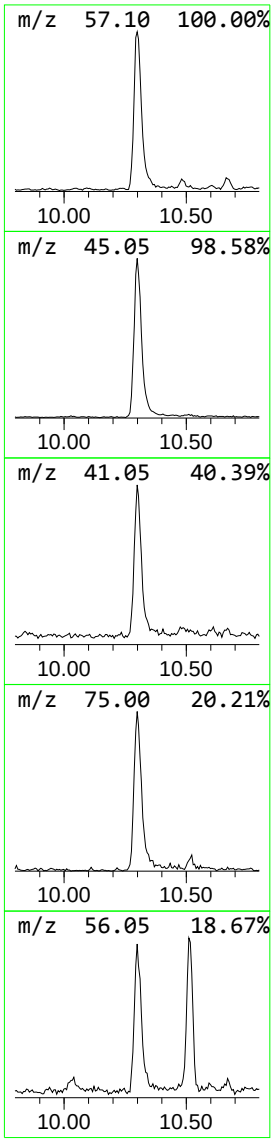
****

Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.299	3.37 ng	296876	Naphthalene-d8	10.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	91
2	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
4	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	47
5	Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	47





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Operator : MA/JU
Sample : P2864-01
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Instrument :
BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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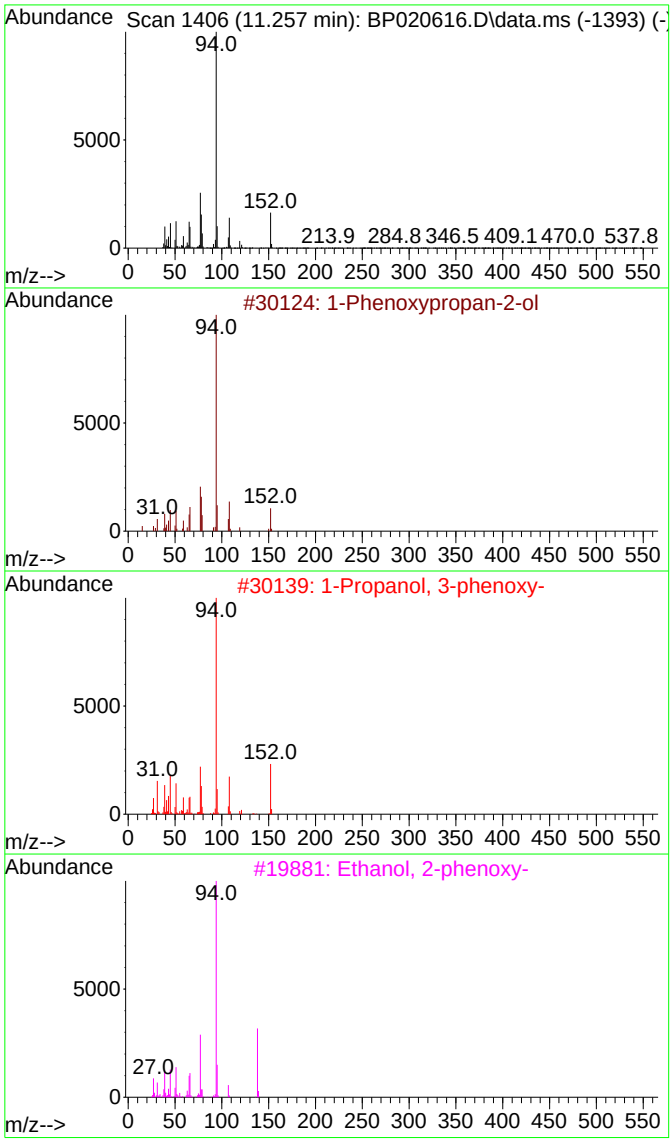
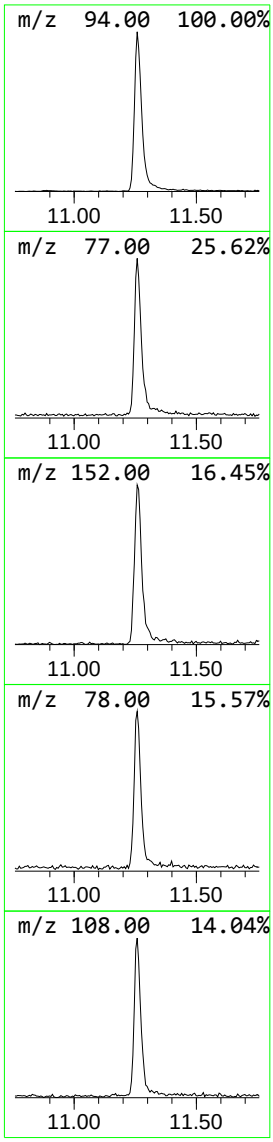
****

Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.257	3.92 ng	345450	Naphthalene-d8	10.516

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	64
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	59
5	Benzene, (1,1-dimethylethoxy)-	150	C10H14O	006669-13-2	53





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Sample : P2864-01
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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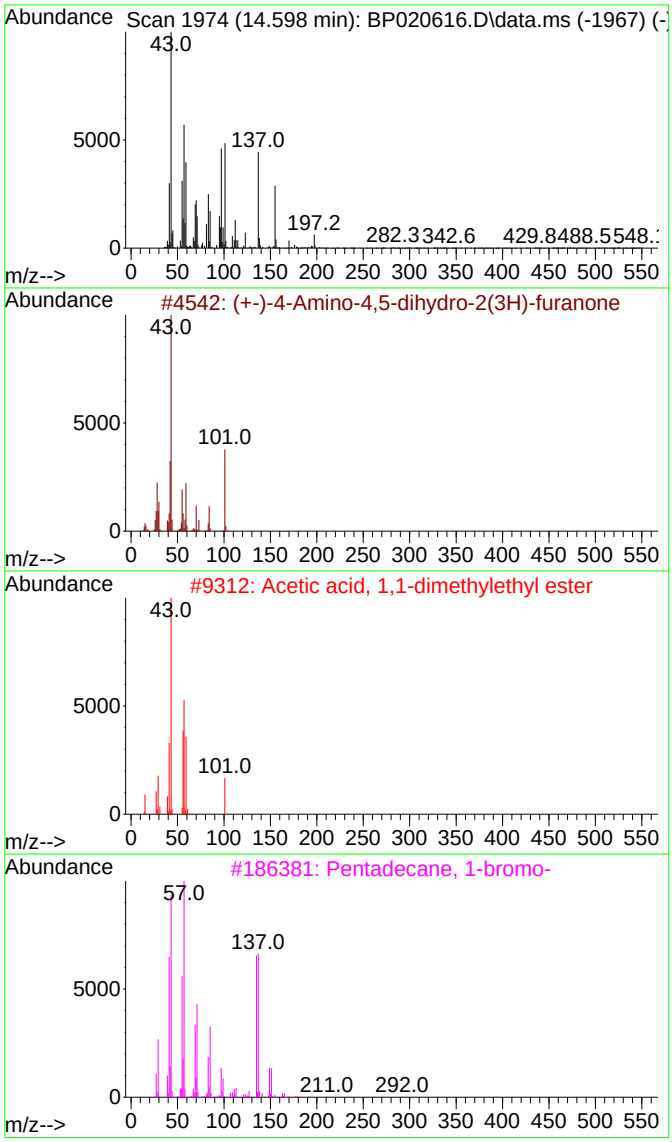
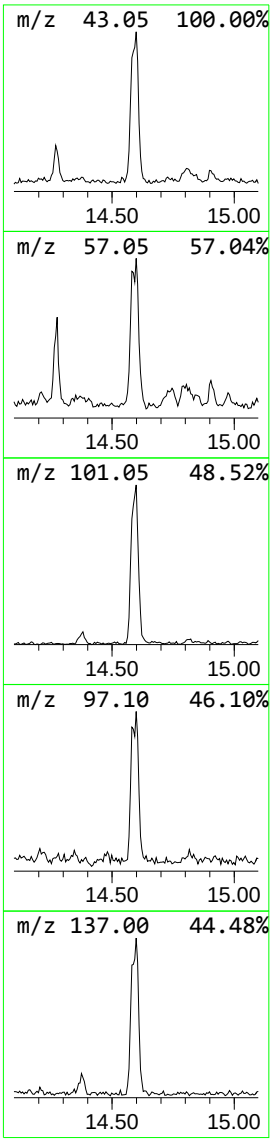
Peak Number 6 unknown14.598 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.598	2.01 ng	239628	Acenaphthene-d10	14.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	22
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	22
3	Pentadecane, 1-bromo-	290	C15H31Br	000629-72-1	10
4	Methyl 3,4,6-tri-O-acetyl-2-acet...	361	C15H23NO9	002595-39-3	10
5	4,7-Dimethyl-5-decyne-4,7-diol	198	C12H22O2	000126-87-4	10





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TIC Library : C:\Database\NIST20.L
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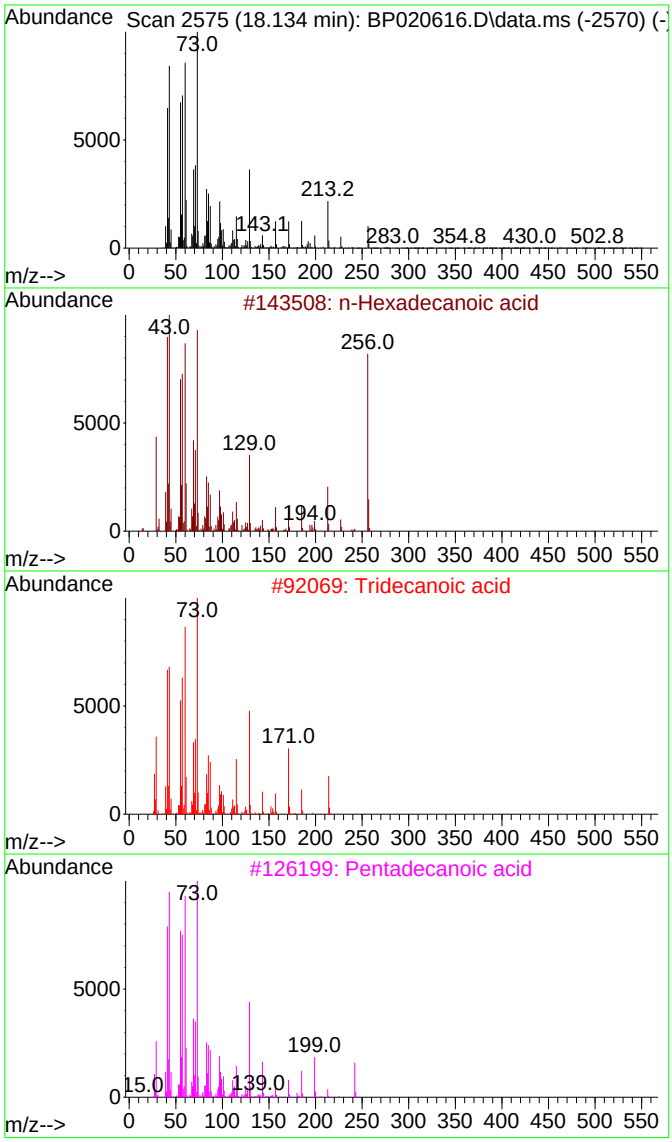
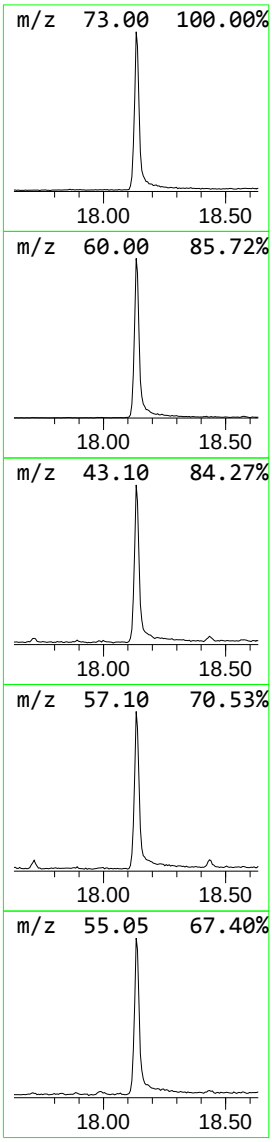
Peak Number 7 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.134	12.58 ng	1783430	Phenanthrene-d10	17.186

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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061324\
Data File : BP020616.D
Acq On : 13 Jun 2024 18:06
Operator : MA/JU
Sample : P2864-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WC-H

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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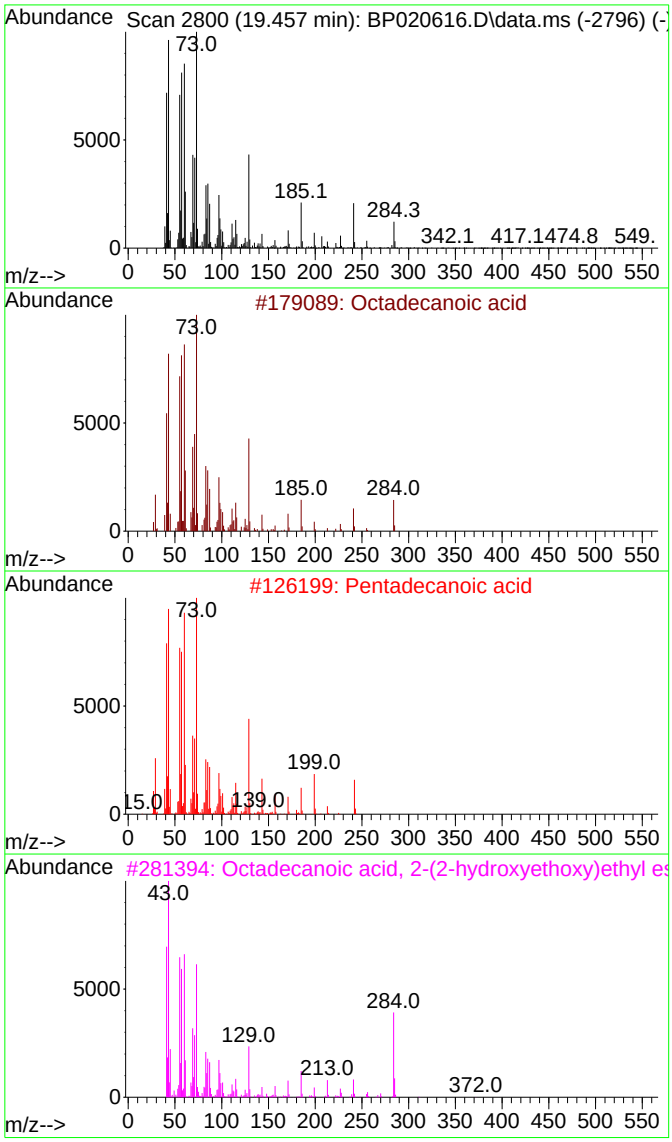
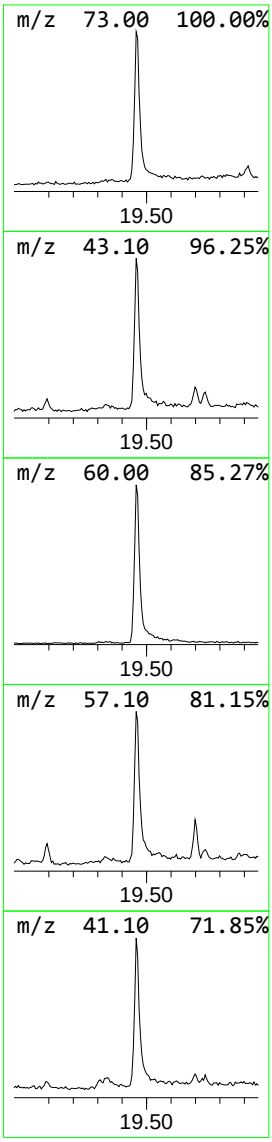
****

Peak Number 8 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.457	5.98 ng	875503	Chrysene-d12	21.645

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	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	83





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Data File : BP020616.D
Acq On : 13 Jun 2024 18:06
Operator : MA/JU
Sample : P2864-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WC-H

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

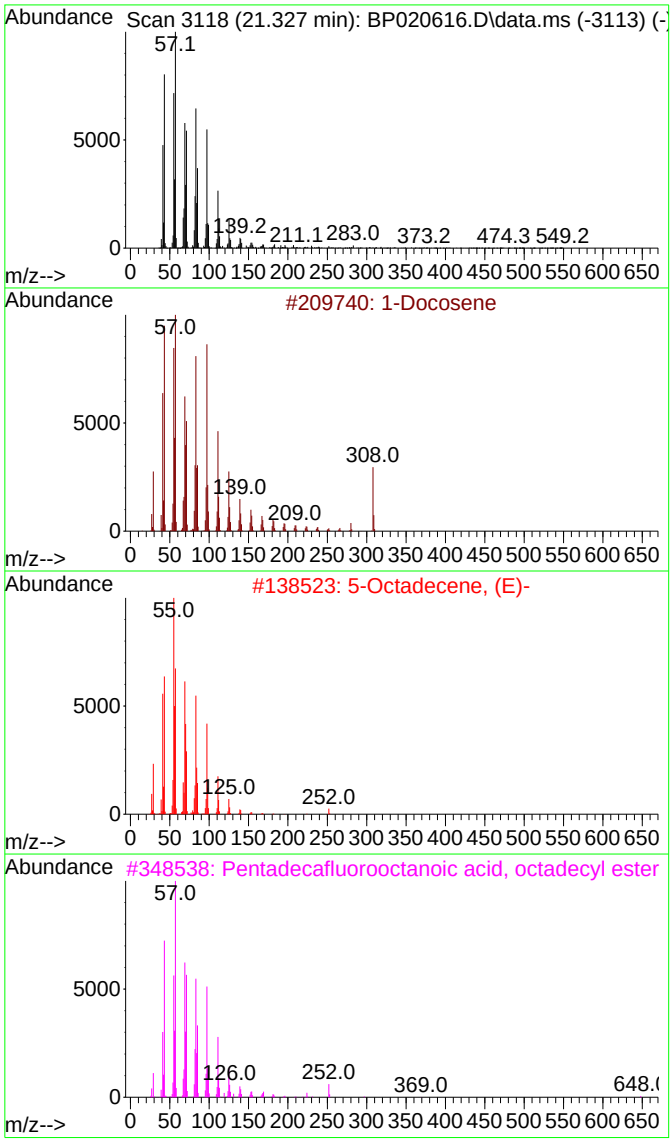
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

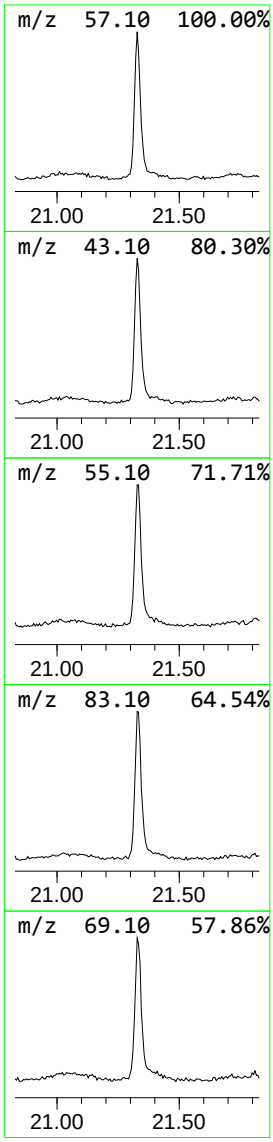
****

Peak Number 9 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.328	8.39 ng	1229700	Chrysene-d12	21.645

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	97
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4	17-Pentatriacontene	491	C35H70	006971-40-0	94
5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061324\
Data File : BP020616.D
Acq On : 13 Jun 2024 18:06
Operator : MA/JU
Sample : P2864-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WC-H

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.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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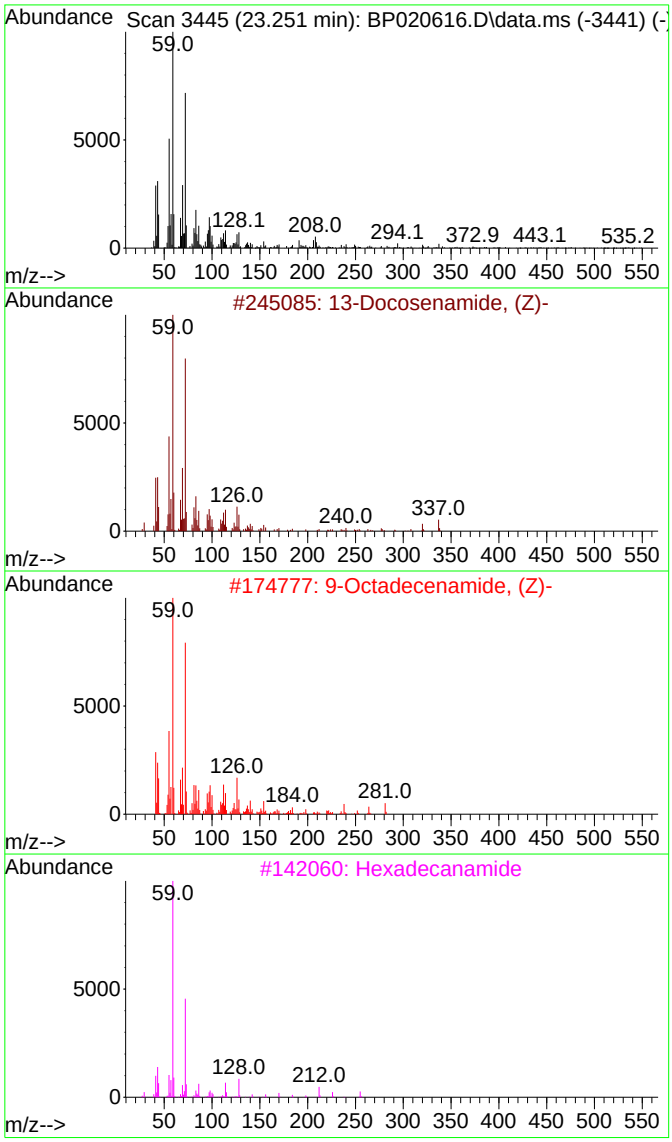
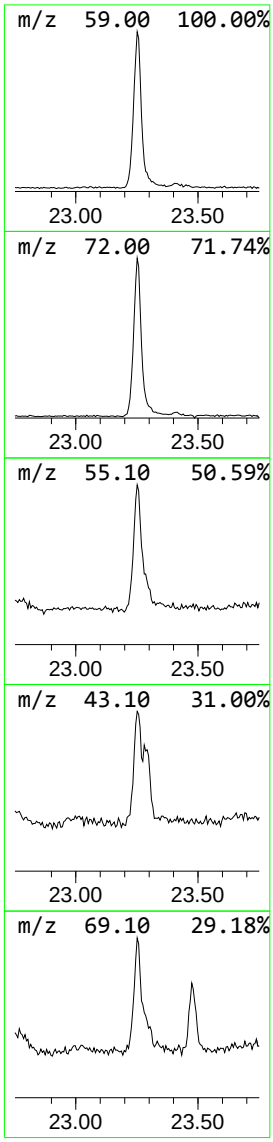
Peak Number 10 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.251	6.47 ng	948088	Chrysene-d12	21.645

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	91
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
3	Hexadecanamide	255	C16H33NO	000629-54-9	72
4	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	59
5	Decanamide-	171	C10H21NO	002319-29-1	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061324\
Data File : BP020616.D
Acq On : 13 Jun 2024 18:06
Operator : MA/JU
Sample : P2864-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WC-H

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.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
Butane, 2-metho...	3.023	46.3	ng	2967680	1	7.752	1283180	20.0
Propylene Glycol	3.552	5.0	ng	321126	1	7.752	1283180	20.0
2-Pentanone, 4-...	4.922	5.5	ng	353576	1	7.752	1283180	20.0
Ethanol, 2-(2-b...	10.299	3.4	ng	296876	2	10.516	1762910	20.0
1-Phenoxypropan...	11.257	3.9	ng	345450	2	10.516	1762910	20.0
unknown14.598	14.598	2.0	ng	239628	3	14.375	2380540	20.0
n-Hexadecanoic ...	18.134	12.6	ng	1783430	4	17.186	2835250	20.0
Octadecanoic acid	19.457	6.0	ng	875503	5	21.645	2929770	20.0
1-Docosene	21.328	8.4	ng	1229700	5	21.645	2929770	20.0
13-Docosenamide...	23.251	6.5	ng	948088	5	21.645	2929770	20.0