LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081721\
Data File : BP006731.D
Acq On : 17 Aug 2021 22:37
Operator : CG/JU
Sample : M3429-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-2

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-BP080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006731.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.852	296	300	309	rVB	97037	149987	1.47%	0.254%
2	5.305	371	377	389	rBV	4158144	5750973	56.40%	9.745%
3	6.887	639	646	659	rVB	3989914	6201812	60.82%	10.509%
4	7.699	778	784	794	rVB	730666	1125639	11.04%	1.907%
5	8.858	974	981	993	rVB	2432537	4055183	39.77%	6.871%
6	10.281	1217	1223	1240	rBV	676535	1152959	11.31%	1.954%
7	10.481	1250	1257	1270	rVB	1000493	1649302	16.18%	2.795%
8	12.963	1672	1679	1688	rBV	5520214	7922887	77.70%	13.425%
9	14.340	1905	1913	1921	rBV	1394611	2001199	19.63%	3.391%
10	15.840	2153	2168	2180	rBV	4500916	6210257	60.91%	10.523%
11	16.098	2205	2212	2217	rBV	101230	144379	1.42%	0.245%
12	16.192	2222	2228	2232	rBV	242498	330353	3.24%	0.560%
13	16.251	2232	2238	2244	rVV2	272825	535141	5.25%	0.907%
14	16.310	2244	2248	2252	rVV2	251844	380140	3.73%	0.644%
15	16.351	2252	2255	2260	rVB	138793	189405	1.86%	0.321%
16	16.510	2277	2282	2289	rVB4	180343	330290	3.24%	0.560%
17	16.581	2289	2294	2298	rBV	244185	340205	3.34%	0.576%
18	16.651	2303	2306	2312	rVB2	137710	186506	1.83%	0.316%
19	17.098	2375	2382	2387	rBV	1645928	2286477	22.42%	3.874%
20	17.139	2387	2389	2396	rVB2	71524	121032	1.19%	0.205%
21	17.792	2495	2500	2507	rBV	137873	157179	1.54%	0.266%
22	18.010	2533	2537	2546	rBV2	151901	217077	2.13%	0.368%
23	18.933	2686	2694	2701	rVB3	150770	224272	2.20%	0.380%
24	19.122	2720	2726	2732	rBV	228218	326035	3.20%	0.552%
25	19.469	2777	2785	2788	rBV	225476	351662	3.45%	0.596%
26	19.504	2788	2791	2796	rVB	208325	261562	2.57%	0.443%
27	19.681	2815	2821	2826	rBV	8533402	10196295	100.00%	17.277%
28	20.939	3031	3035	3042	rBV3	256713	436813	4.28%	0.740%
29	21.204	3074	3080	3084	rVV	1985779	2668391	26.17%	4.522%
30	21.239	3084	3086	3093	rVB	147586	175138	1.72%	0.297%
31	21.845	3186	3189	3198	rVB3	148997	232255	2.28%	0.394%
32	23.516	3466	3473	3489	rVB2	1346002	2704438	26.52%	4.583%

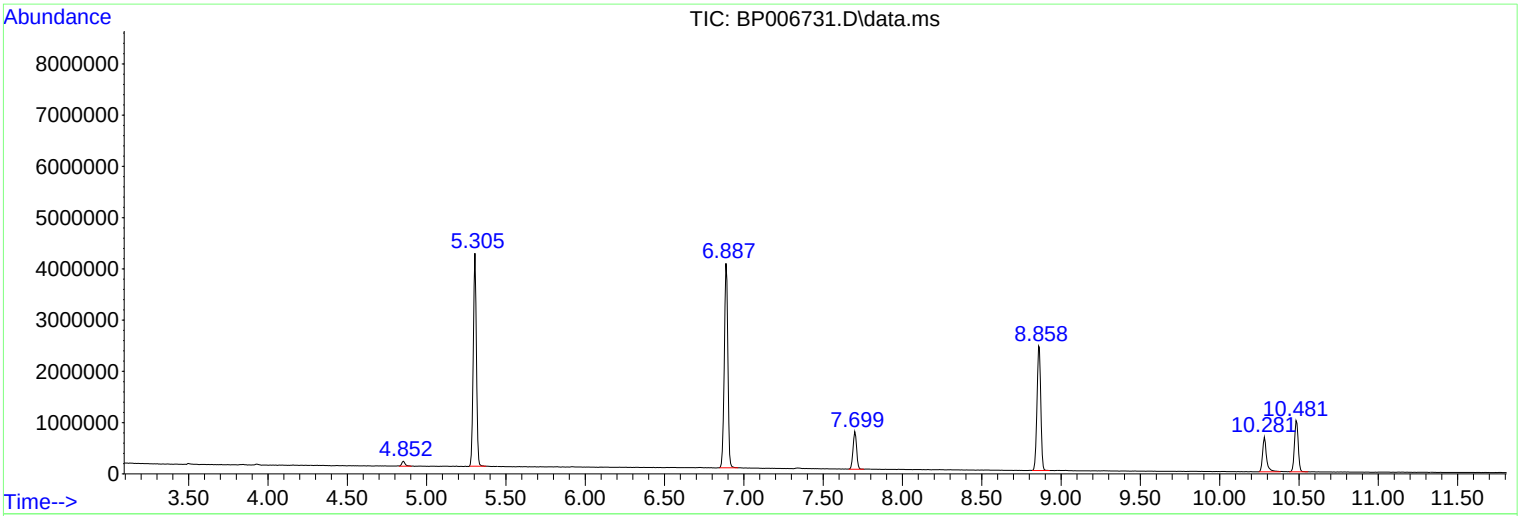
Sum of corrected areas: 59015243

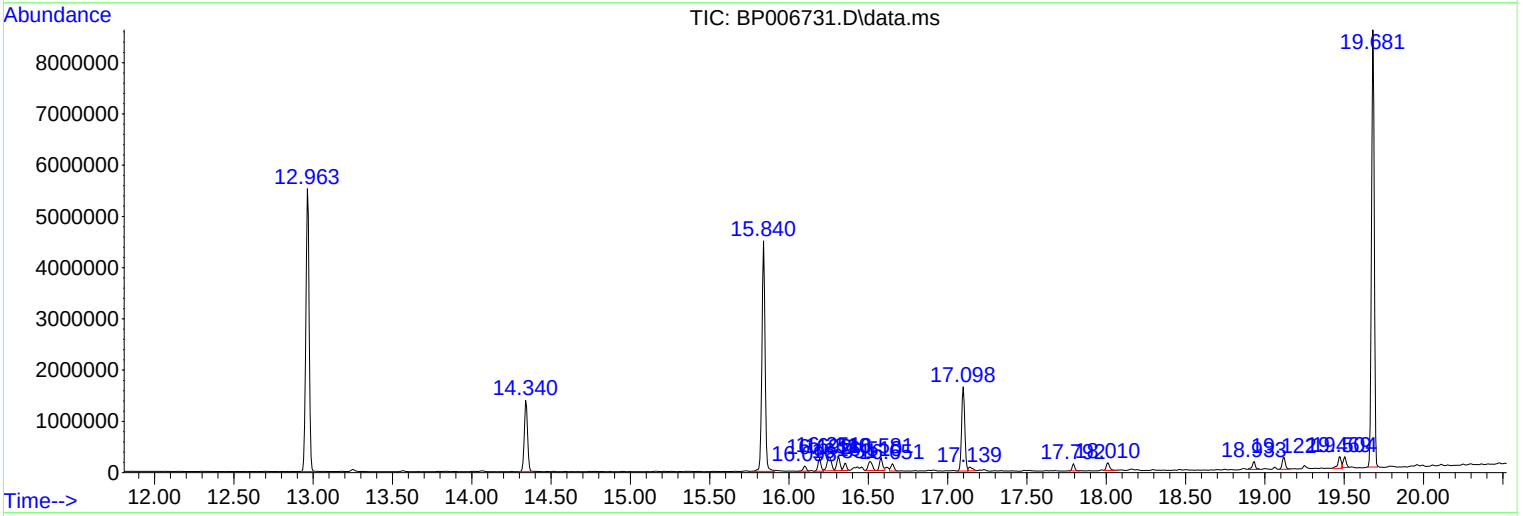
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081721\
Data File : BP006731.D
Acq On : 17 Aug 2021 22:37
Operator : CG/JU
Sample : M3429-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

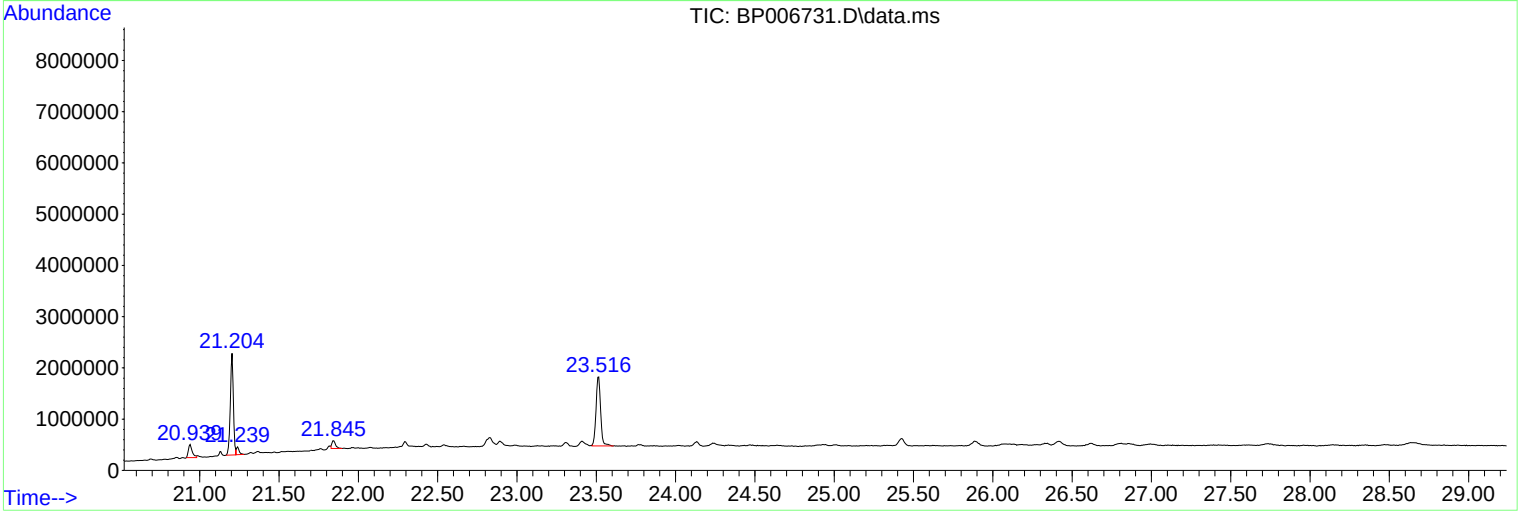
Instrument :
BNA_P
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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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Data File : BP006731.D
Acq On : 17 Aug 2021 22:37
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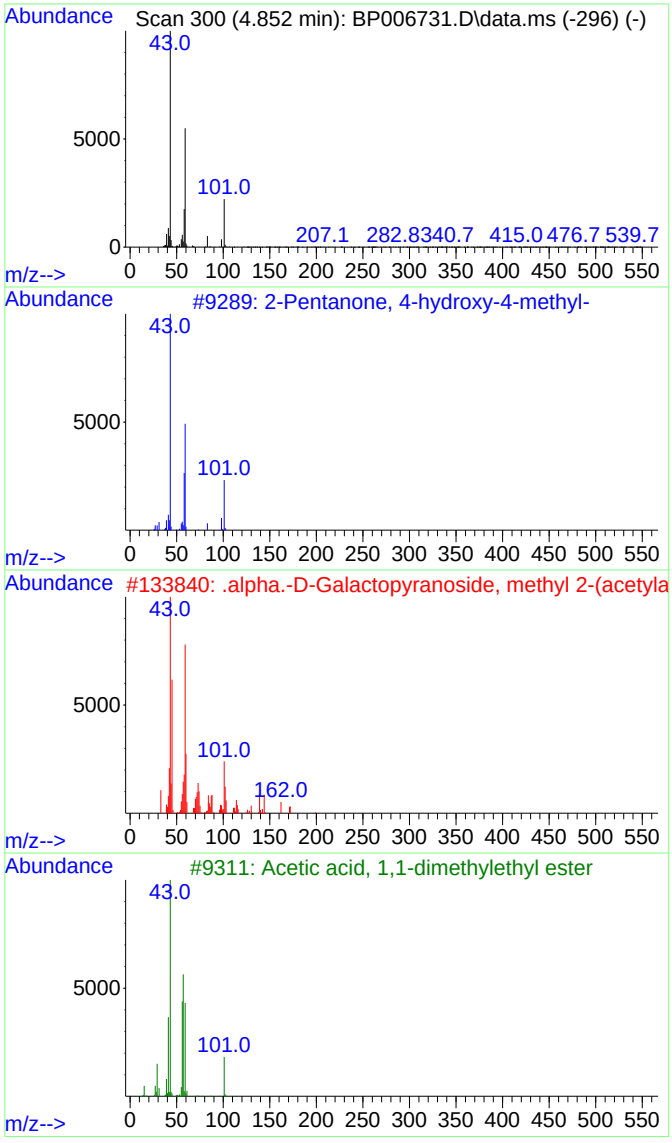
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

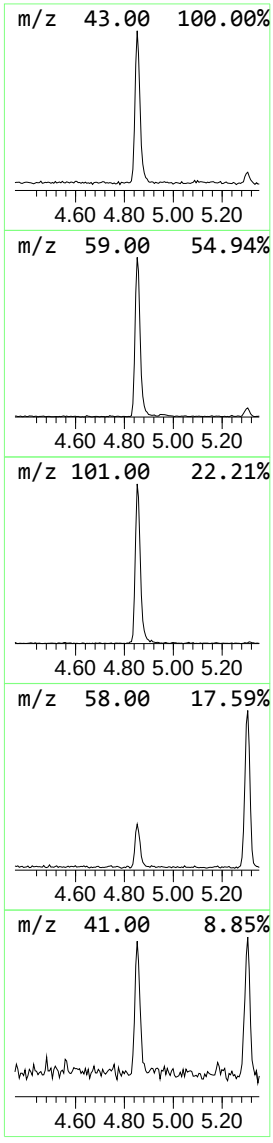
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.852	2.66 ng	149987	1,4-Dichlorobenzene-d4	7.699

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	.alpha.-D-Galactopyranoside, met...	249	C10H19NO6	017296-07-0	38
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081721\
Data File : BP006731.D
Acq On : 17 Aug 2021 22:37
Operator : CG/JU
Sample : M3429-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-2

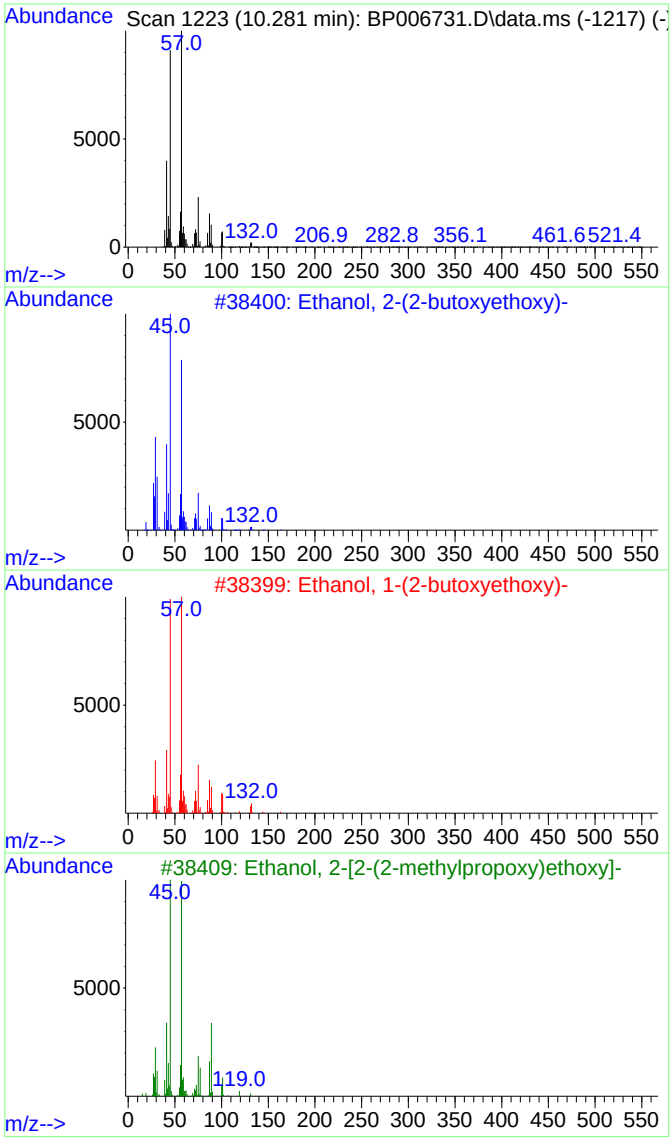
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

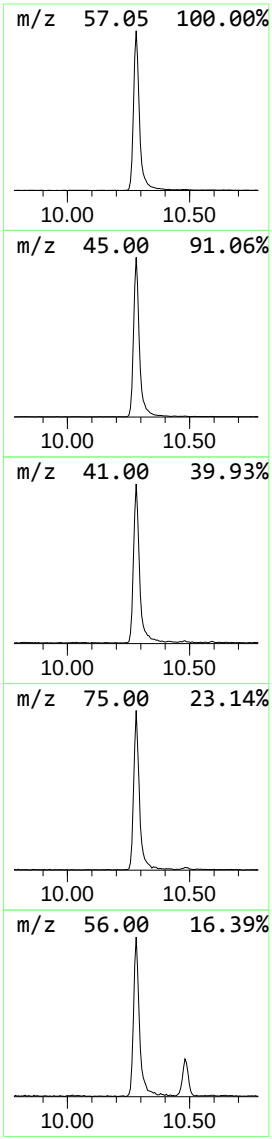
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.281	13.98 ng	1152960	Naphthalene-d8	10.481

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50





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Data File : BP006731.D
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Operator : CG/JU
Sample : M3429-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WC-2

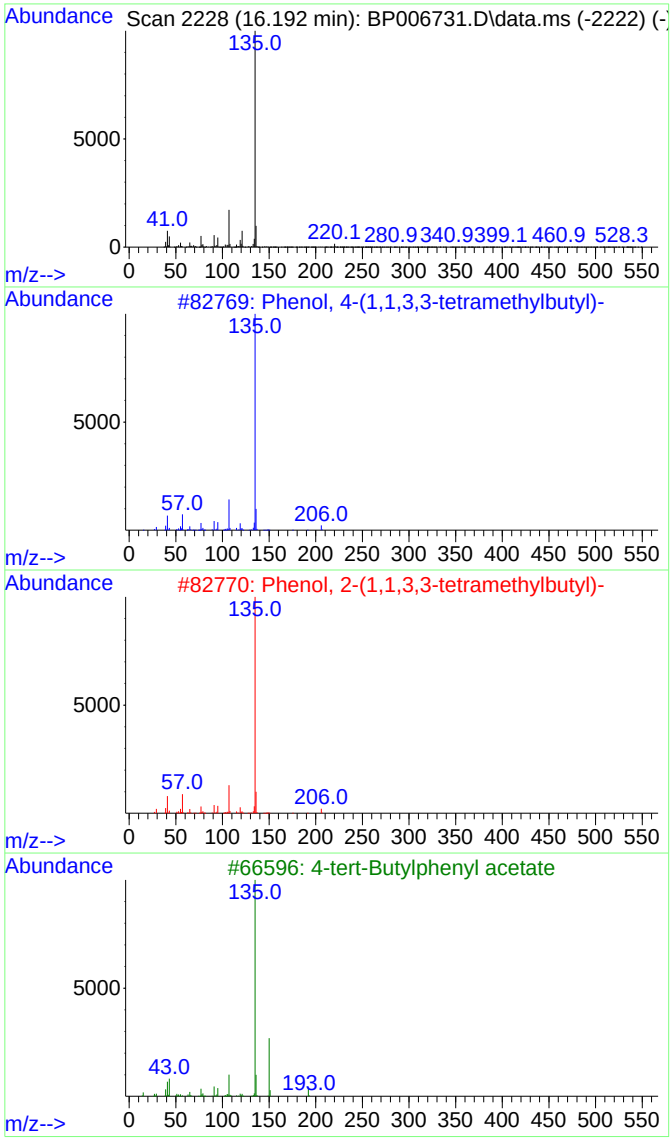
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

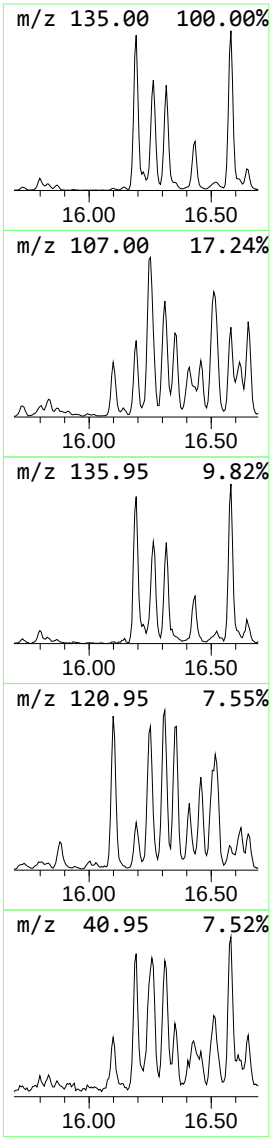
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Phenol, 4-(1,1,3,3-tetramet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.192	2.89 ng	330353	Phenanthrene-d10	17.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	86
2	Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	78
3	4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	78
4	4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	78
5	2-tert-Butylphenol, O-(n-propylo...	236	C14H20O3	1000487-37-9	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081721\
Data File : BP006731.D
Acq On : 17 Aug 2021 22:37
Operator : CG/JU
Sample : M3429-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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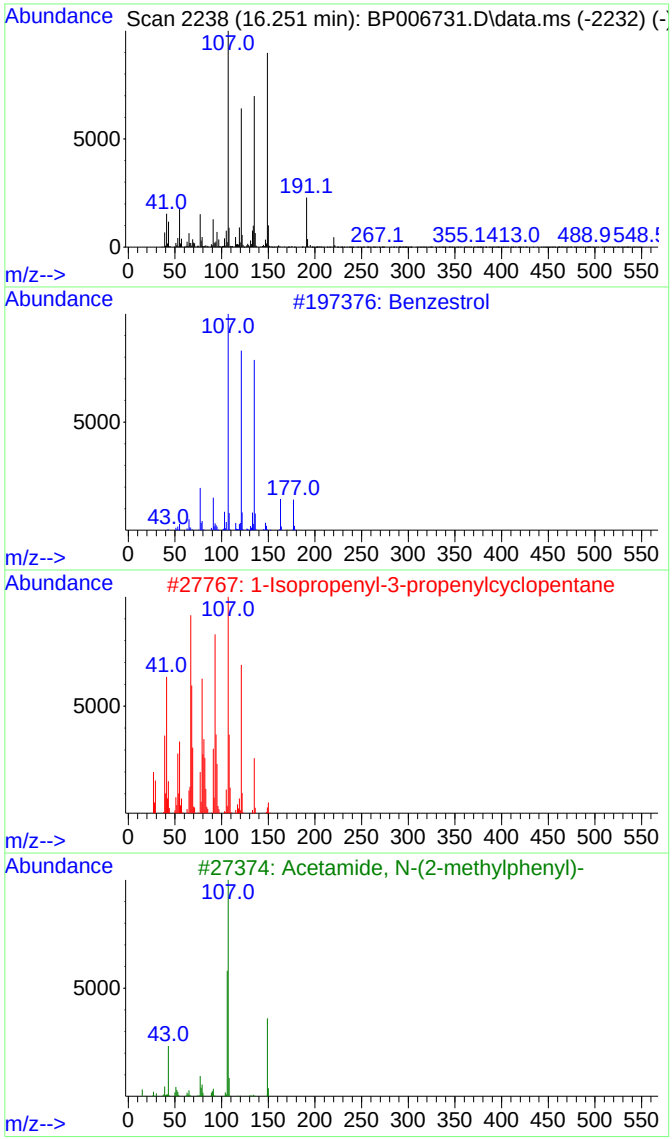
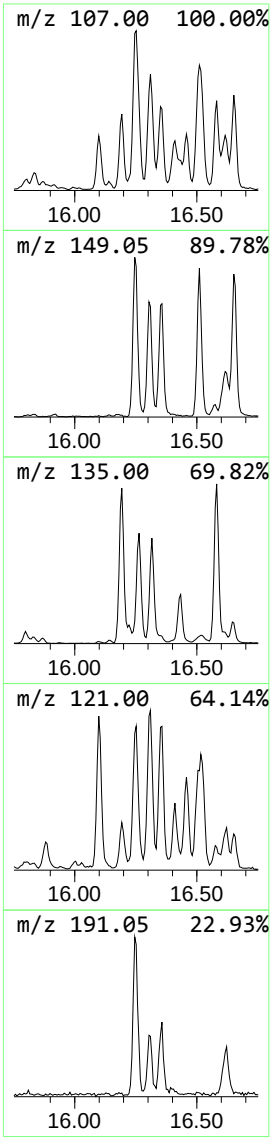
****

Peak Number 4 unknown16.251 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.251	4.68 ng	535141	Phenanthrene-d10	17.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzestrol	298	C20H26O2	000085-95-0	43
2	1-Isopropenyl-3-propenylcyclopen...	150	C11H18	1000192-81-2	38
3	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	35
4	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	000103-89-9	27
5	Gardamide	191	C12H17NO	084434-18-4	27





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Operator : CG/JU
Sample : M3429-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

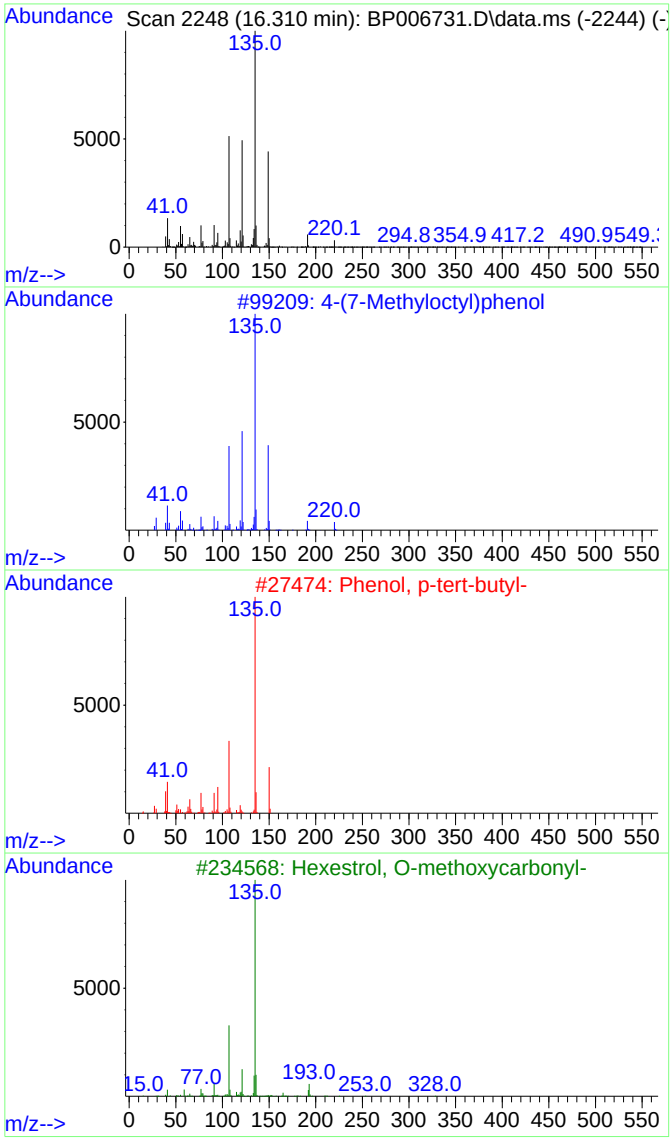
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

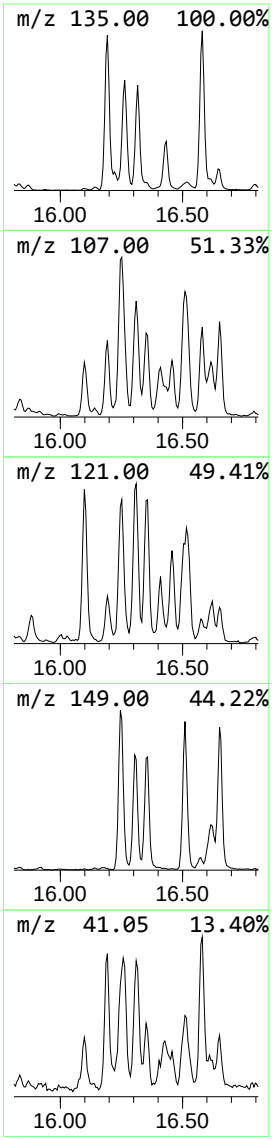
****

Peak Number 5 4-(7-Methyloctyl)phenol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.310	3.33 ng	380140	Phenanthrene-d10	17.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(7-Methyloctyl)phenol	220	C15H24O	024518-48-7	98
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	64
3	Hexestrol, O-methoxycarbonyl-	328	C20H24O4	1000487-66-3	53
4	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	50
5	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	50





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Sample : M3429-04
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Instrument : BNA_P
ClientSampleId : WC-2

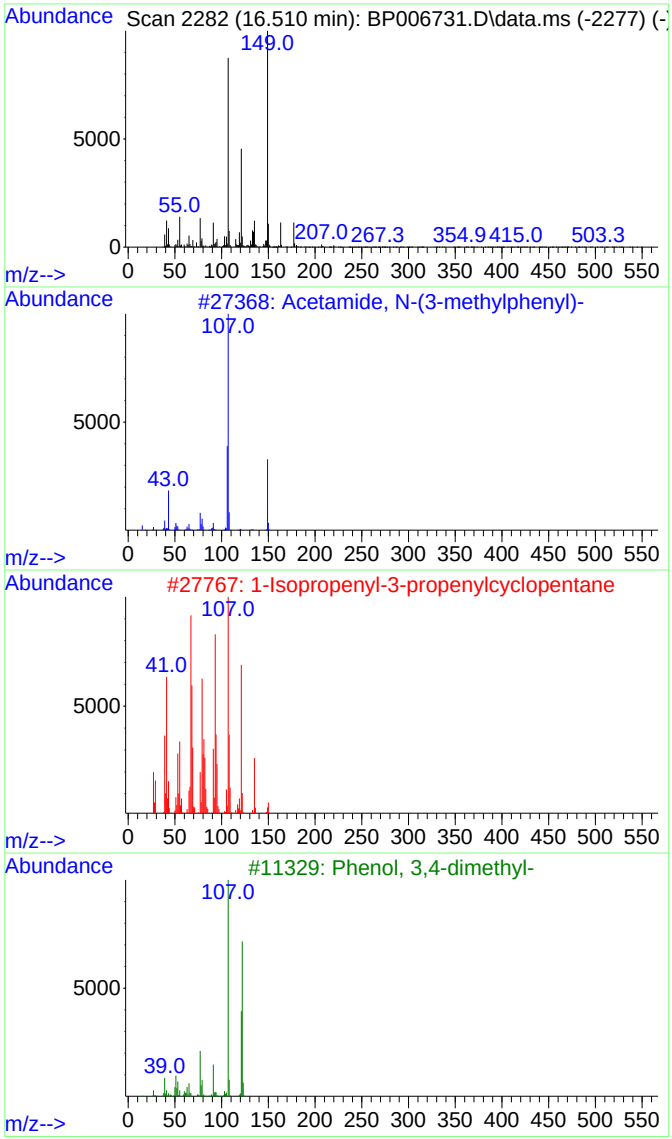
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

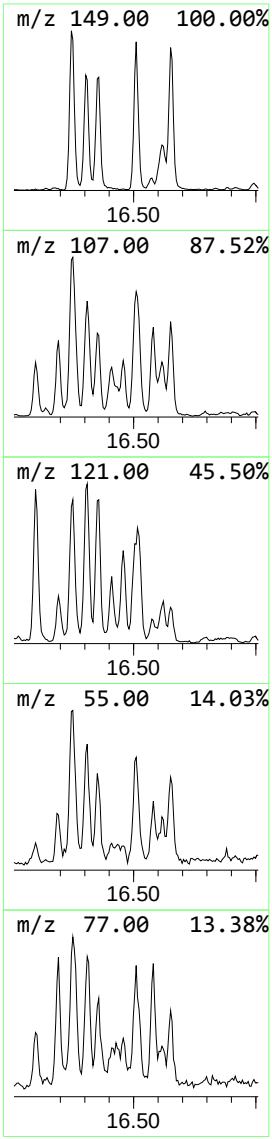
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Acetamide, N-(3-methylphenyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.510	2.89 ng	330290	Phenanthrene-d10	17.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	59
2	1-Isopropenyl-3-propenylcyclopen...	150	C11H18	1000192-81-2	50
3	Phenol, 3,4-dimethyl-	122	C8H10O	000095-65-8	38
4	2-(Heptyloxycarbonyl)benzoic acid	264	C15H20O4	024539-58-0	38
5	3,4-(methylenedioxy)-phenylbutan...	192	C11H12O3	1000378-99-2	38





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Acq On : 17 Aug 2021 22:37
Operator : CG/JU
Sample : M3429-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-2

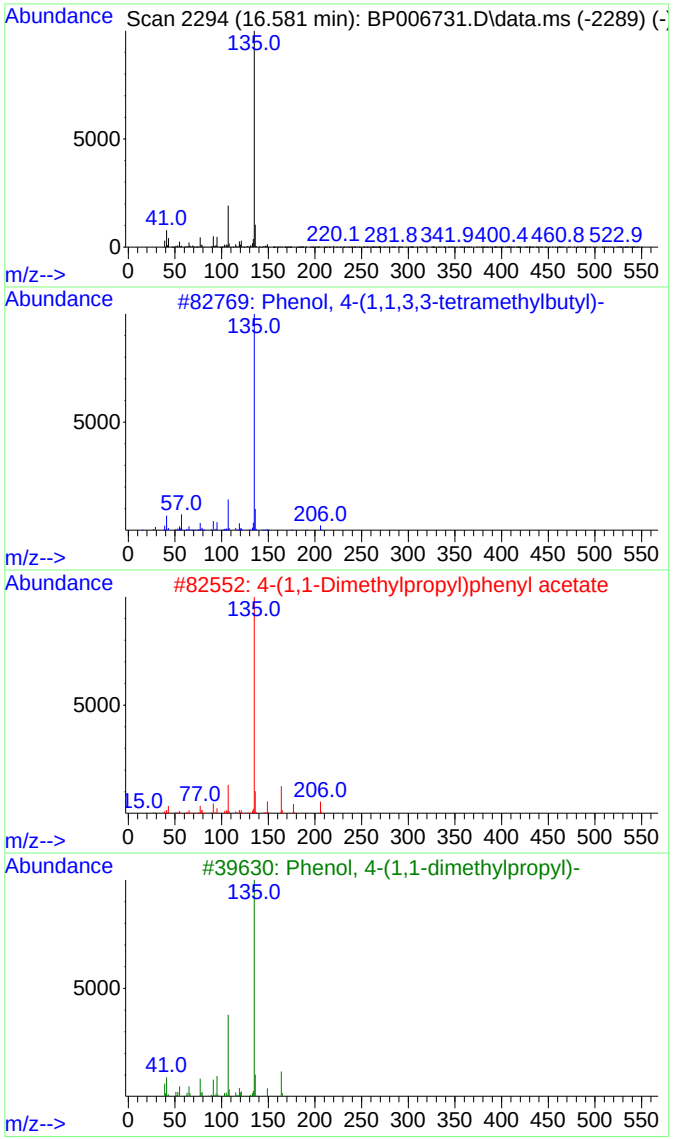
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

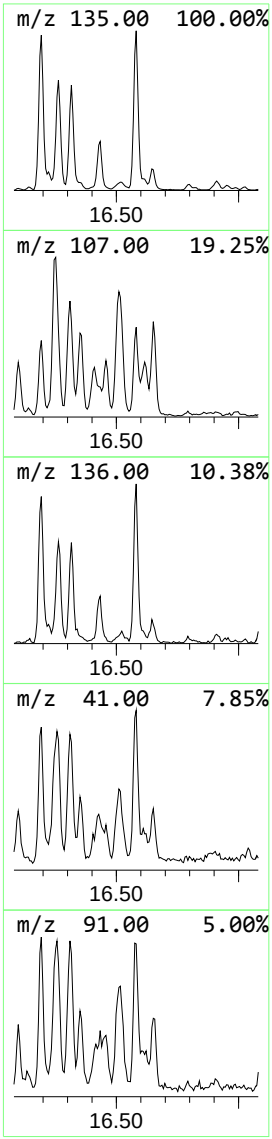
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4-(1,1-Dimethylpropyl)pheny... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.581	2.98 ng	340205	Phenanthrene-d10	17.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	86
2	4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	83
3	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	78
4	Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	78
5	Hexestrol	270	C18H22O2	000084-16-2	72





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Sample : M3429-04
Misc :
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Instrument : BNA_P
ClientSampleId : WC-2

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

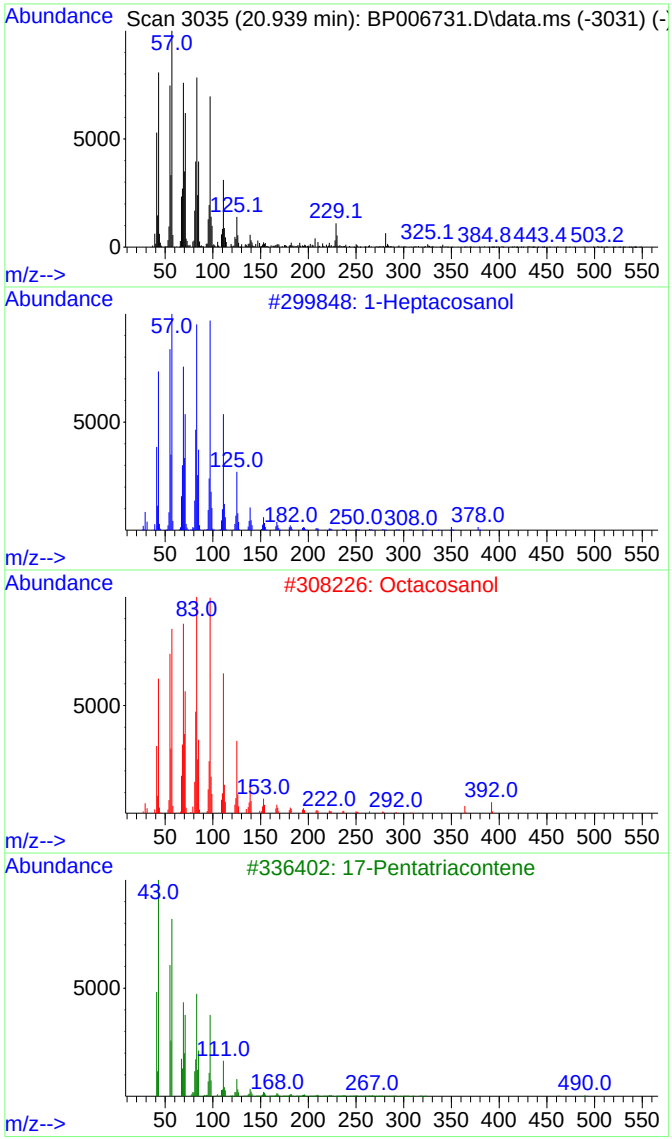
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

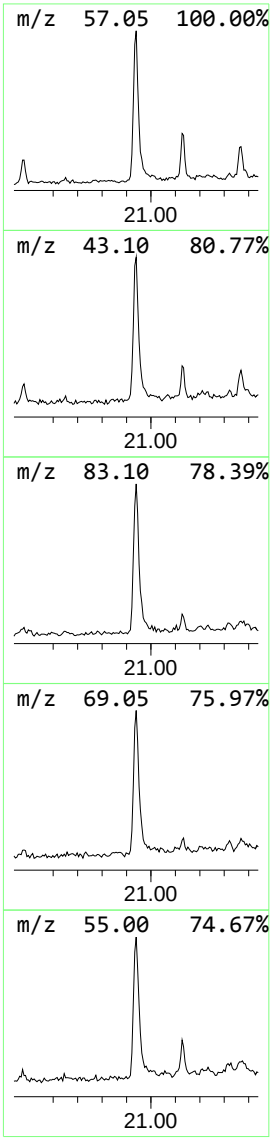
****

Peak Number 8 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.939	3.27 ng	436813	Chrysene-d12	21.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	Octacosanol	410	C28H58O	000557-61-9	91
3	17-Pentatriacontene	491	C35H70	006971-40-0	91
4	1-Hexacosanol	382	C26H54O	000506-52-5	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081721\
Data File : BP006731.D
Acq On : 17 Aug 2021 22:37
Operator : CG/JU
Sample : M3429-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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-...	4.852	2.7	ng	149987	1	7.699	1125640	20.0
Ethanol, 2-(2-b...	10.281	14.0	ng	1152960	2	10.481	1649300	20.0
Phenol, 4-(1,1,...	16.192	2.9	ng	330353	4	17.098	2286480	20.0
unknown16.251	16.251	4.7	ng	535141	4	17.098	2286480	20.0
4-(7-Methylocty...	16.310	3.3	ng	380140	4	17.098	2286480	20.0
Acetamide, N-(3...	16.510	2.9	ng	330290	4	17.098	2286480	20.0
4-(1,1-Dimethyl...	16.581	3.0	ng	340205	4	17.098	2286480	20.0
1-Heptacosanol	20.939	3.3	ng	436813	5	21.204	2668390	20.0