LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051421\
Data File : BP005550.D
Acq On : 14 May 2021 15:52
Operator : CG/JU
Sample : M2373-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : OR-02-051221

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-BP050521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005550.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.269	364	371	386	rBV	85115	128982	6.84%	1.707%
2	6.875	638	644	657	rBV	67107	123463	6.54%	1.634%
3	7.675	771	780	787	rBV	66719	104905	5.56%	1.388%
4	8.845	971	979	986	rBV	50281	86458	4.58%	1.144%
5	10.469	1246	1255	1261	rBV	72279	118741	6.29%	1.572%
6	12.945	1670	1676	1683	rVB	146989	216519	11.48%	2.866%
7	13.798	1815	1821	1828	rBV	15580	26267	1.39%	0.348%
8	14.328	1906	1911	1918	rVB	120800	173058	9.17%	2.291%
9	15.833	2158	2167	2175	rBV	161455	240027	12.72%	3.177%
10	16.504	2275	2281	2290	rBV5	21075	45069	2.39%	0.597%
11	16.757	2316	2324	2332	rVB5	14074	42771	2.27%	0.566%
12	17.086	2374	2380	2384	rBV	166808	231213	12.26%	3.060%
13	17.127	2384	2387	2395	rVV	49244	73883	3.92%	0.978%
14	17.221	2399	2403	2408	rVB	17071	24314	1.29%	0.322%
15	17.763	2490	2495	2499	rBV7	12446	20463	1.08%	0.271%
16	17.992	2530	2534	2541	rVV4	52826	95985	5.09%	1.270%
17	18.121	2542	2556	2569	rVV	159437	652432	34.58%	8.635%
18	18.274	2570	2582	2593	rVV	308468	965772	51.19%	12.782%
19	18.410	2593	2605	2617	rVB	708519	1886494	100.00%	24.969%
20	18.557	2625	2630	2639	rVB	55800	121723	6.45%	1.611%
21	18.851	2676	2680	2684	rBV3	14193	23199	1.23%	0.307%
22	19.110	2719	2724	2730	rBV	105953	141140	7.48%	1.868%
23	19.227	2740	2744	2748	rBV4	30358	44463	2.36%	0.588%
24	19.315	2753	2759	2767	rVB3	48335	104612	5.55%	1.385%
25	19.463	2776	2784	2793	rVB	96911	162305	8.60%	2.148%
26	19.539	2793	2797	2804	rBV10	11725	26200	1.39%	0.347%
27	19.657	2813	2817	2822	rVB	369932	430810	22.84%	5.702%
28	20.139	2895	2899	2908	rVB3	64050	131262	6.96%	1.737%
29	20.845	3015	3019	3025	rBV3	95467	146436	7.76%	1.938%
30	21.186	3071	3077	3081	rBV2	280536	423101	22.43%	5.600%
31	21.221	3081	3083	3093	rVB	60434	84098	4.46%	1.113%
32	21.474	3123	3126	3136	rVB2	87805	133498	7.08%	1.767%
33	23.498	3465	3470	3476	rVB2	176247	325794	17.27%	4.312%

Sum of corrected areas: 7555457

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051421\
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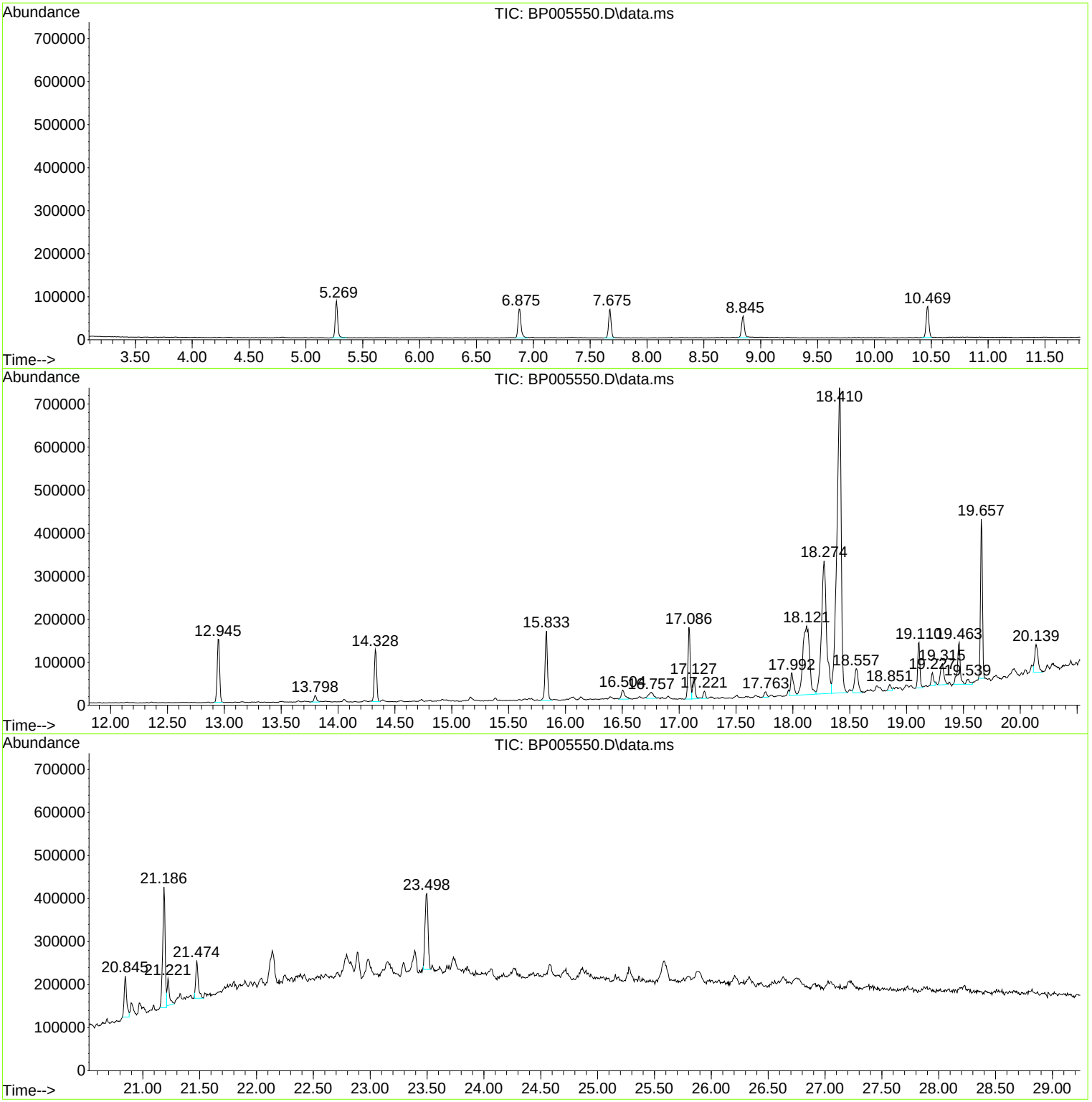
Operator : CG/JU
Sample : M2373-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
OR-02-051221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051421\
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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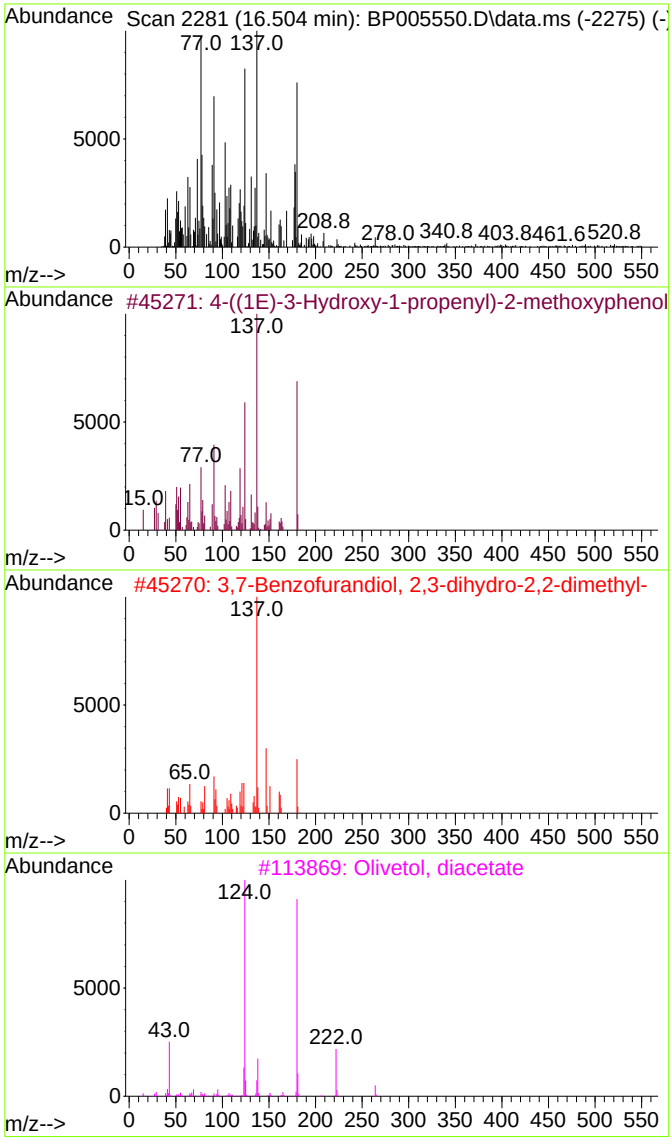
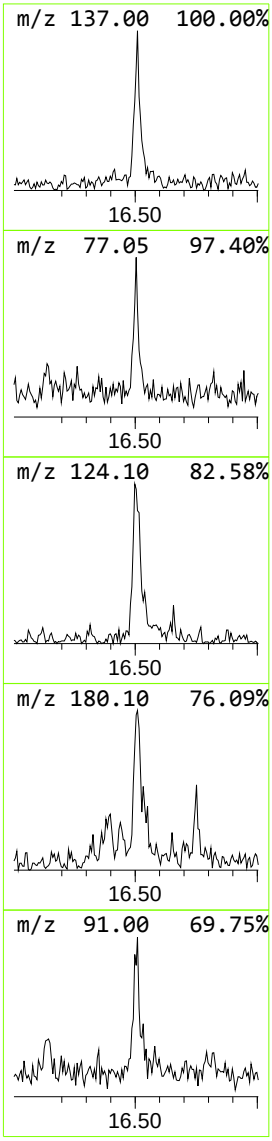
Peak Number 1 unknown16.50 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.504	3.90 ng	45069	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-((1E)-3-Hydroxy-1-propenyl)-2-...	180	C10H12O3	1000297-95-5	43
2	3,7-Benzofurandiol, 2,3-dihydro-...	180	C10H12O3	017781-15-6	38
3	Olivetol, diacetate	264	C15H20O4	1000364-90-9	25
4	Benzene, 1-(butylthio)-4-methyl-	180	C11H16S	021784-96-3	25
5	1,3-Benzenediol, 5-pentyl-	180	C11H16O2	000500-66-3	25





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Data File : BP005550.D
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Operator : CG/JU
Sample : M2373-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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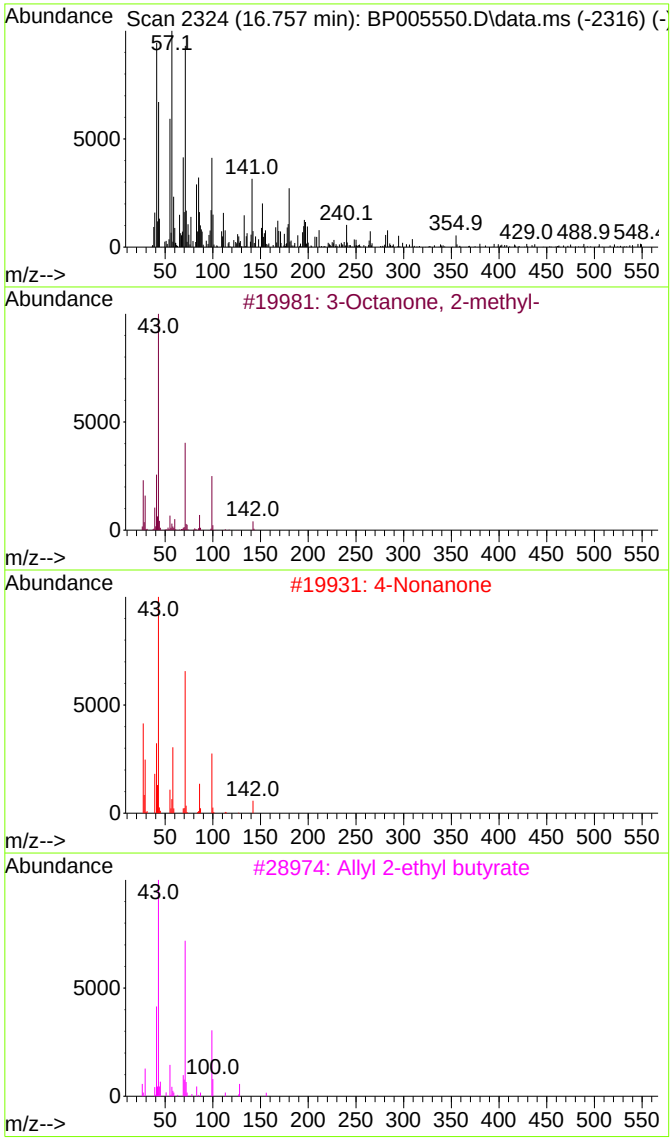
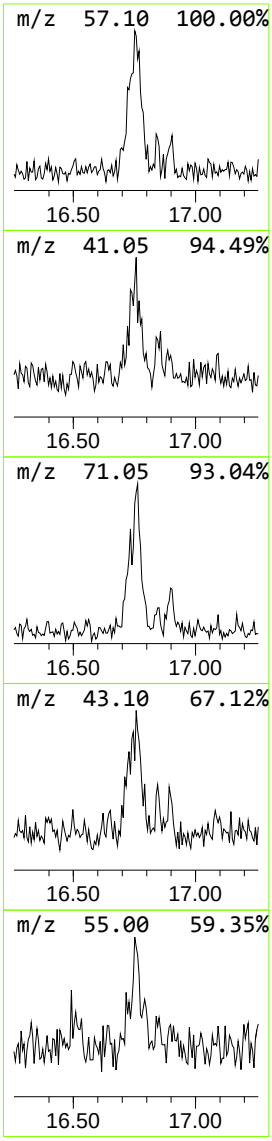
Peak Number 2 3-Octanone, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.757	3.70 ng	42771	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone, 2-methyl-	142	C9H18O	000923-28-4	58
2	4-Nonanone	142	C9H18O	004485-09-0	58
3	Allyl 2-ethyl butyrate	156	C9H16O2	007493-69-8	53
4	Heptadecane	240	C17H36	000629-78-7	47
5	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	43





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Operator : CG/JU
Sample : M2373-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
OR-02-051221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
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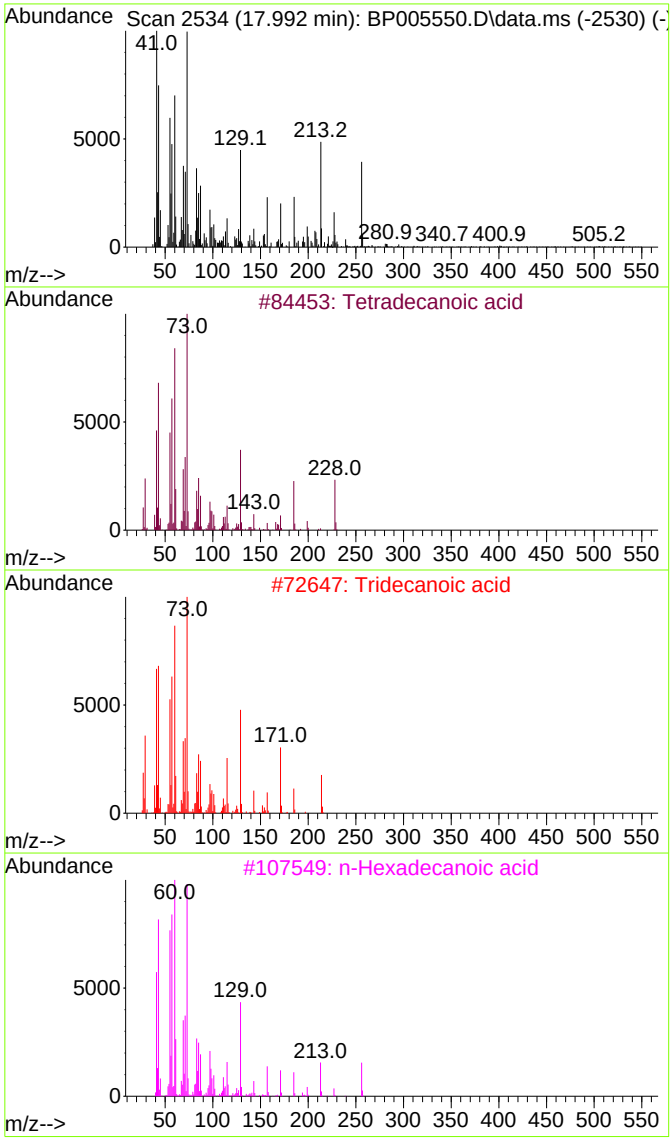
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

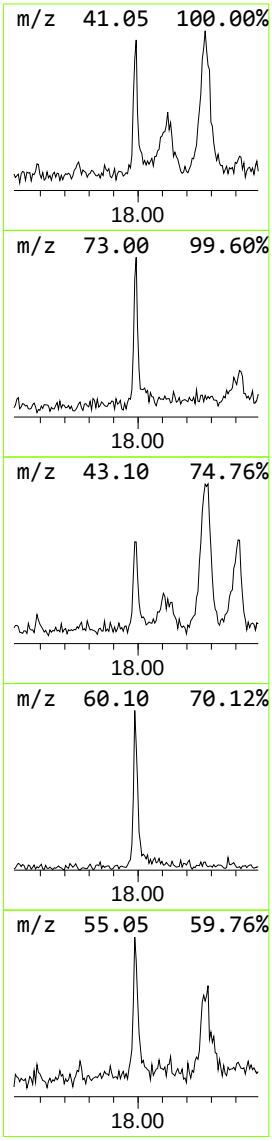
****

Peak Number 3 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.992	8.30 ng	95985	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
2	Tridecanoic acid	214	C13H26O2	000638-53-9	78
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
4	Dodecanoic acid	200	C12H24O2	000143-07-7	52
5	Isopropyl palmitate	298	C19H38O2	000142-91-6	43





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Data File : BP005550.D
Acq On : 14 May 2021 15:52
Operator : CG/JU
Sample : M2373-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
OR-02-051221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

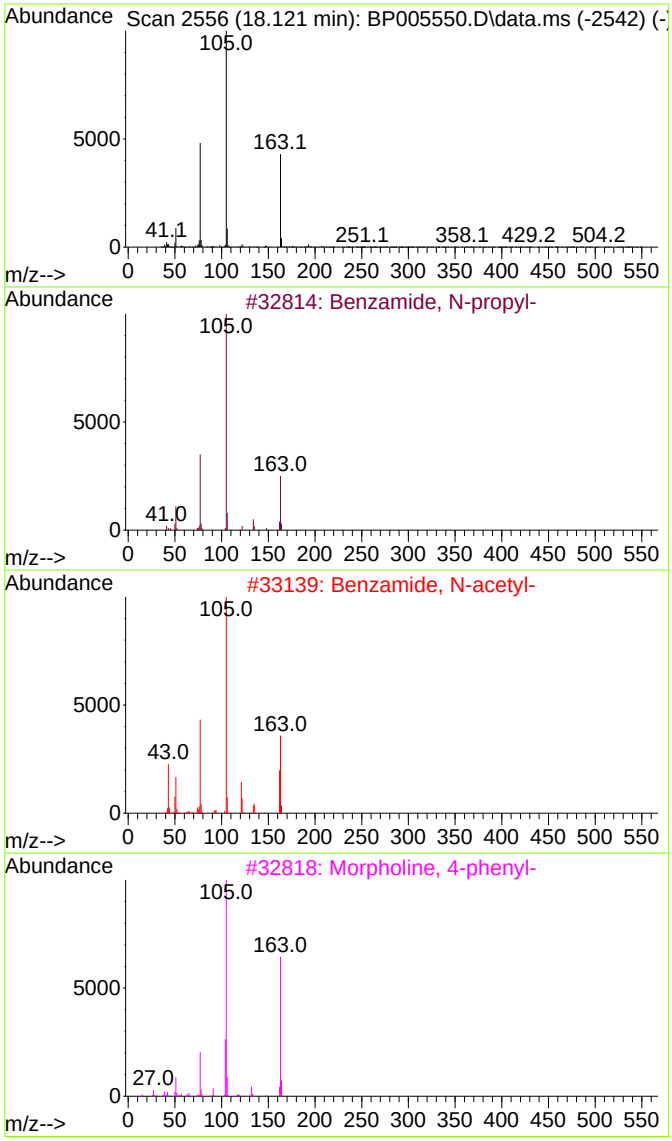
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

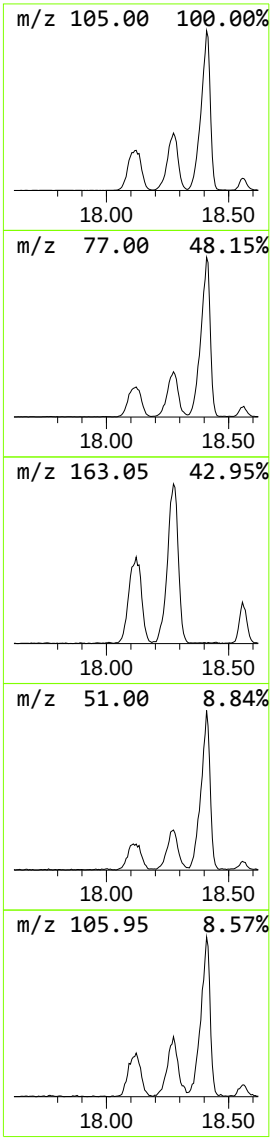
****

Peak Number 4 Benzamide, N-propyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.121	56.44 ng	652432	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	78
2	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	64
3	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	43
4	1,2-Propanedione, 1-phenyl-, 2-o...	163	C9H9NO2	000119-51-7	9
5	(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051421\
Data File : BP005550.D
Acq On : 14 May 2021 15:52
Operator : CG/JU
Sample : M2373-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
OR-02-051221

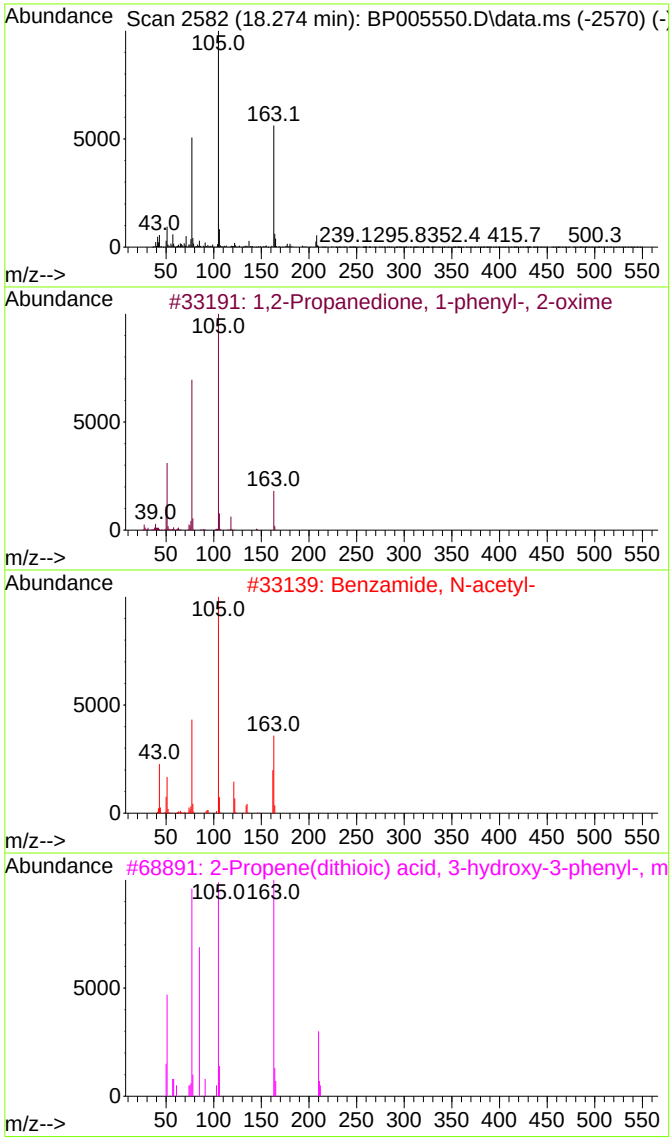
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

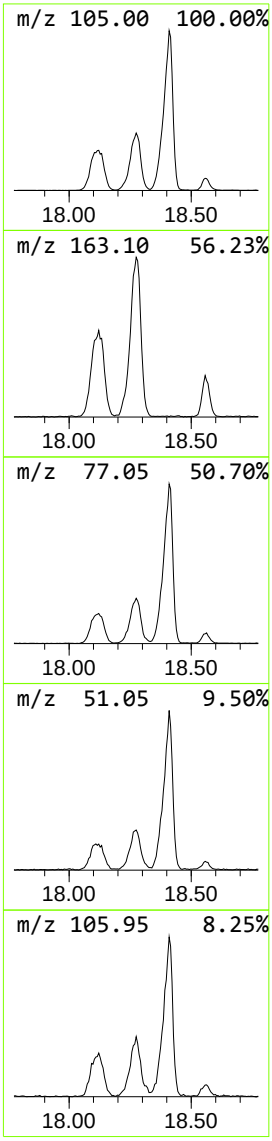
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,2-Propanedione, 1-phenyl-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.274	83.54 ng	965772	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Propanedione, 1-phenyl-, 2-o...	163	C9H9NO2	000119-51-7	64
2	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	64
3	2-Propene(dithioic) acid, 3-hydr...	210	C10H10OS2	013636-68-5	50
4	2-Propen-1-one, 1,2-diphenyl-	208	C15H12O	004452-11-3	47
5	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	46





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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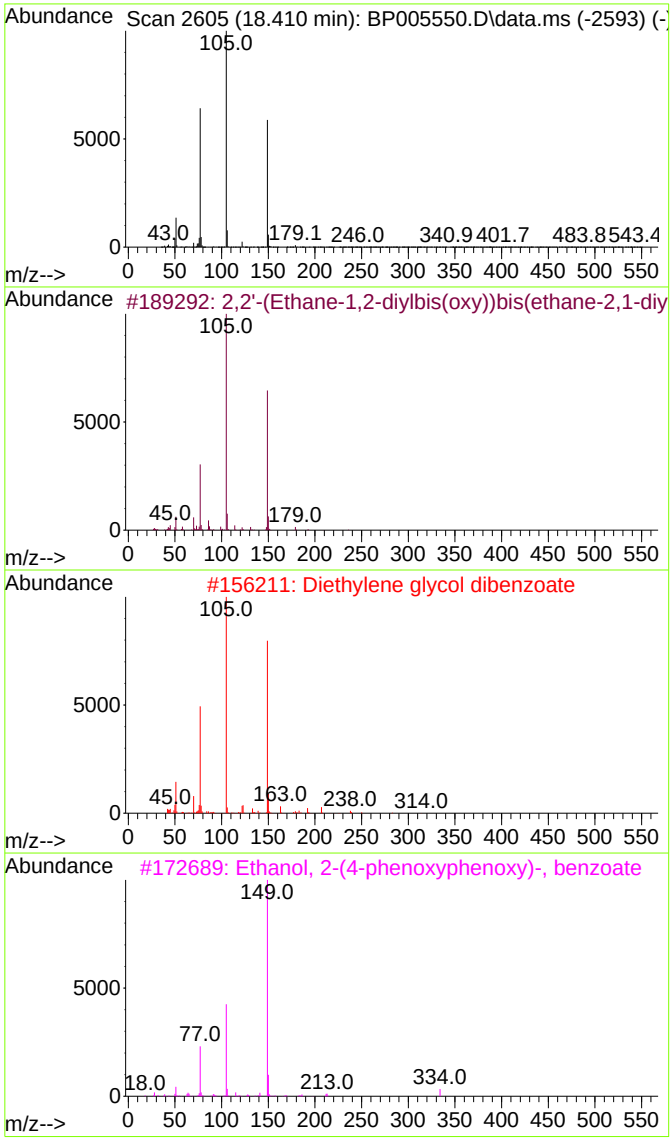
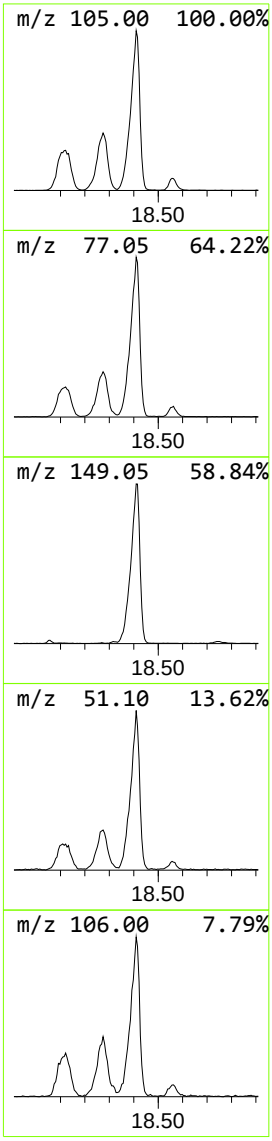
****
Peak Number 6 2,2'-(Ethane-1,2-diylbis(ox... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.410	163.18 ng	1886490	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	83
2	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	74
3	Ethanol, 2-(4-phenoxyphenoxy)-, ...	334	C21H18O4	055191-59-8	64
4	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	64
5	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	50





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Operator : CG/JU
Sample : M2373-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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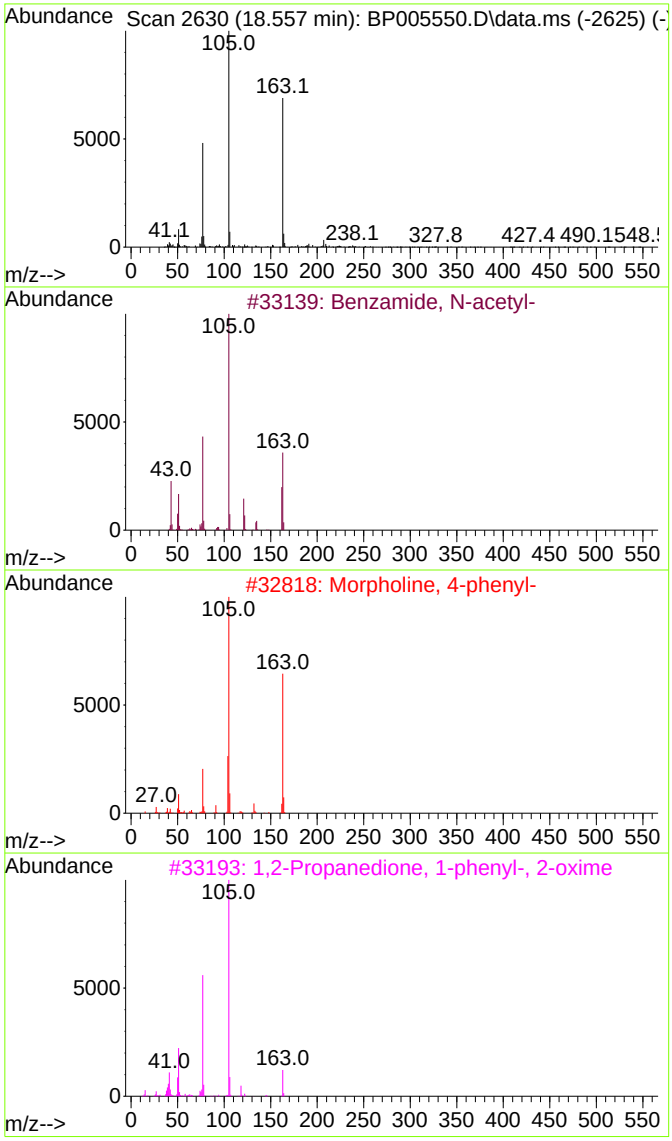
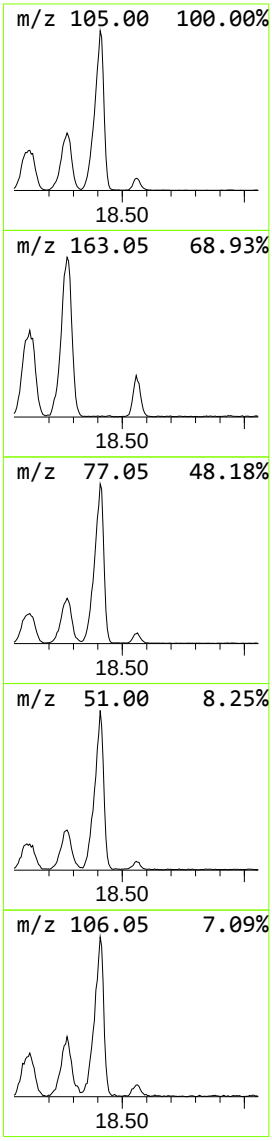
Peak Number 7 Benzamide, N-acetyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.557	10.53 ng	121723	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	64
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	49
3	1,2-Propanedione, 1-phenyl-, 2-o...	163	C9H9NO2	000119-51-7	42
4	Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	40
5	Isoindole-1,3(1H,3H)-dione, 2-et...	191	C10H9NO3	001914-21-2	27





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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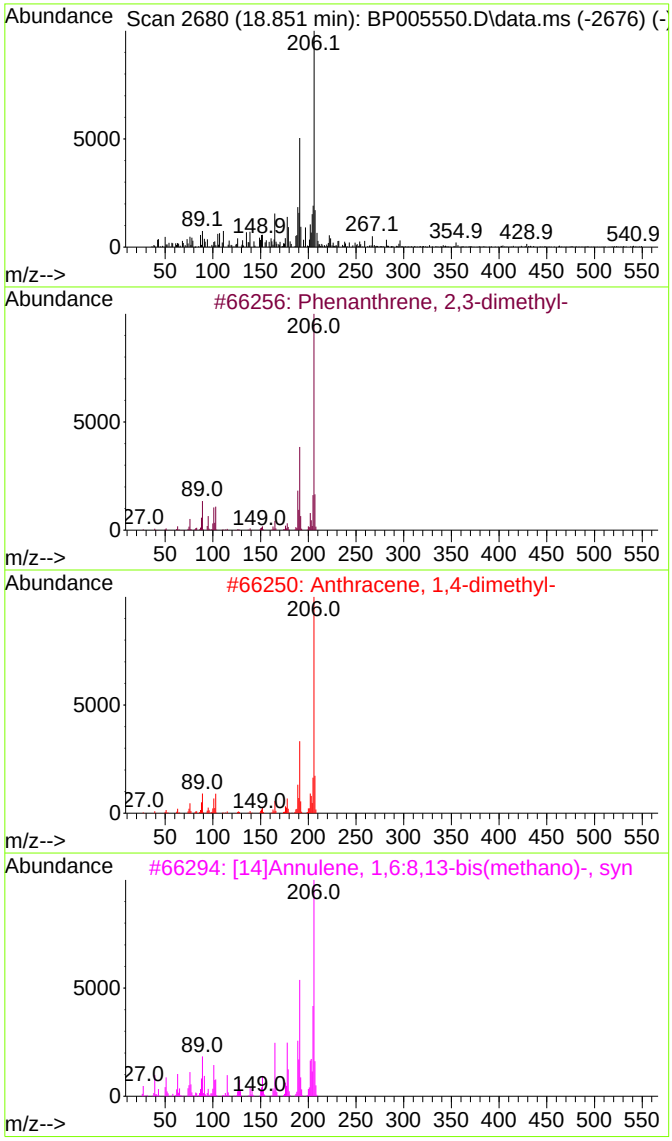
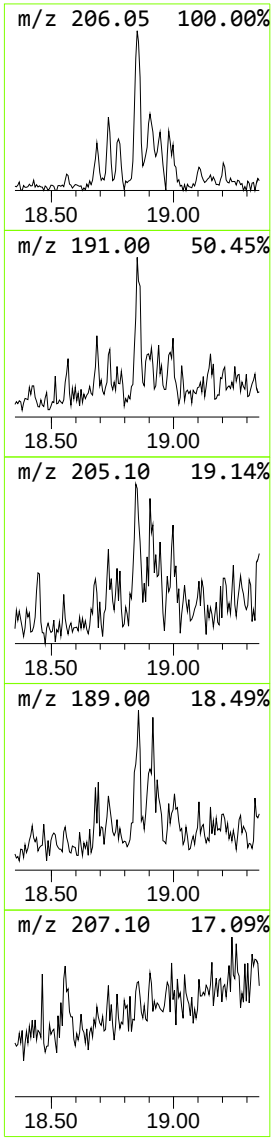
Peak Number 8 Phenanthrene, 2,3-dimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.851	2.01 ng	23199	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	90
2	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	90
3	[14]Annulene, 1,6:8,13-bis(metha...	206	C16H14	085385-68-8	89
4	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	87
5	9,10-Dimethylanthracene	206	C16H14	000781-43-1	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051421\
Data File : BP005550.D
Acq On : 14 May 2021 15:52
Operator : CG/JU
Sample : M2373-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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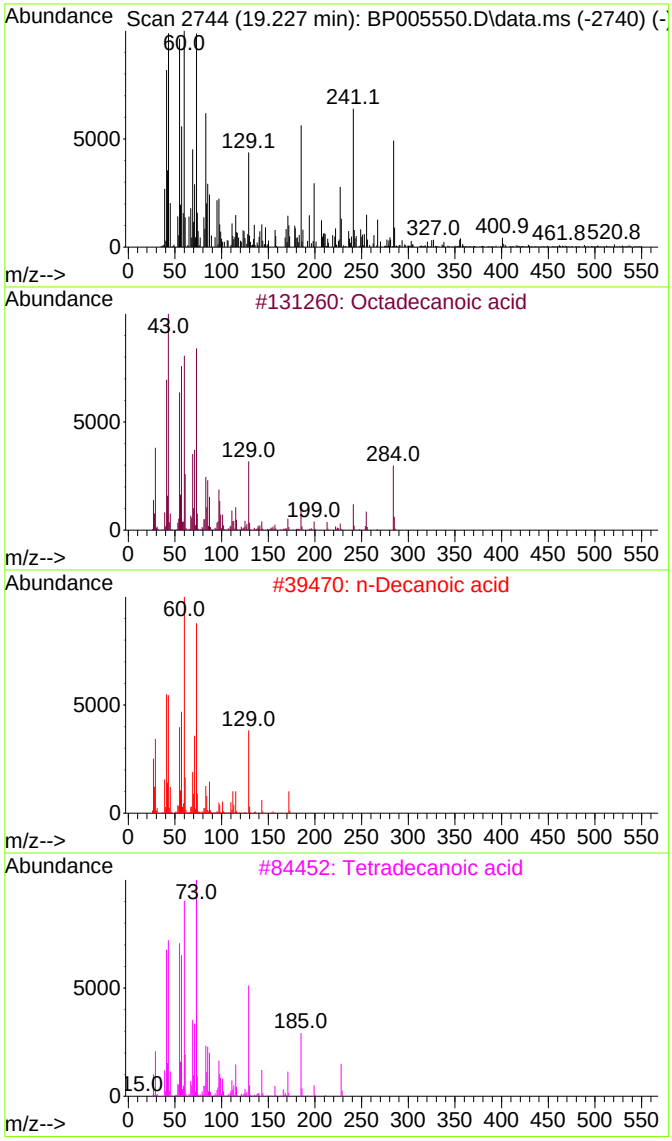
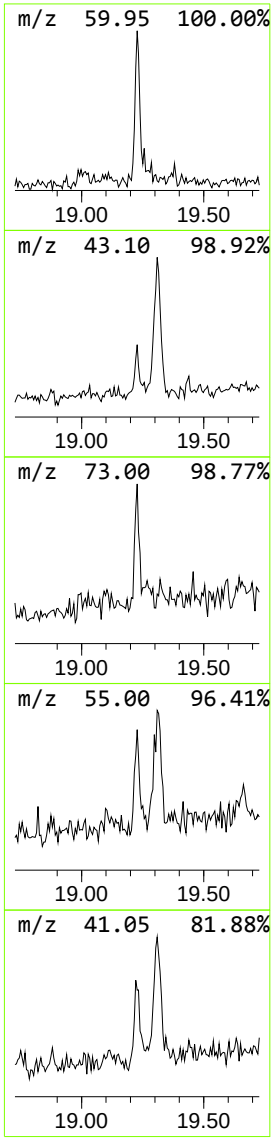
Peak Number 9 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.227	2.10 ng	44463	Chrysene-d12	21.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	78
2	n-Decanoic acid	172	C10H20O2	000334-48-5	42
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	38
4	Dodecanoic acid	200	C12H24O2	000143-07-7	30
5	Nonanoic acid	158	C9H18O2	000112-05-0	14





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Data File : BP005550.D
Acq On : 14 May 2021 15:52
Operator : CG/JU
Sample : M2373-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
OR-02-051221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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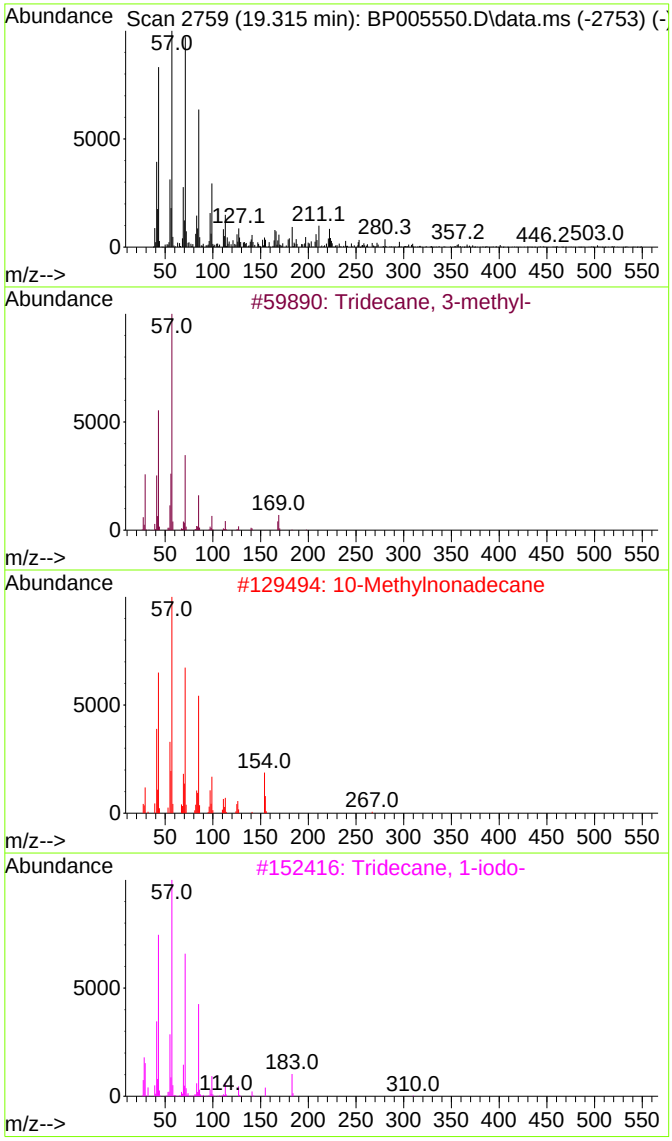
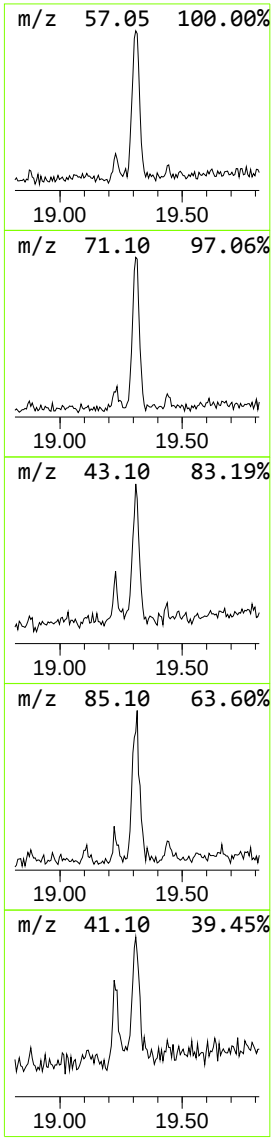
Peak Number 10 Tridecane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.316	4.95 ng	104612	Chrysene-d12	21.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 3-methyl-	198	C14H30	006418-41-3	83
2	10-Methylnonadecane	282	C20H42	056862-62-5	83
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	81
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	80
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80





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Operator : CG/JU
Sample : M2373-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
OR-02-051221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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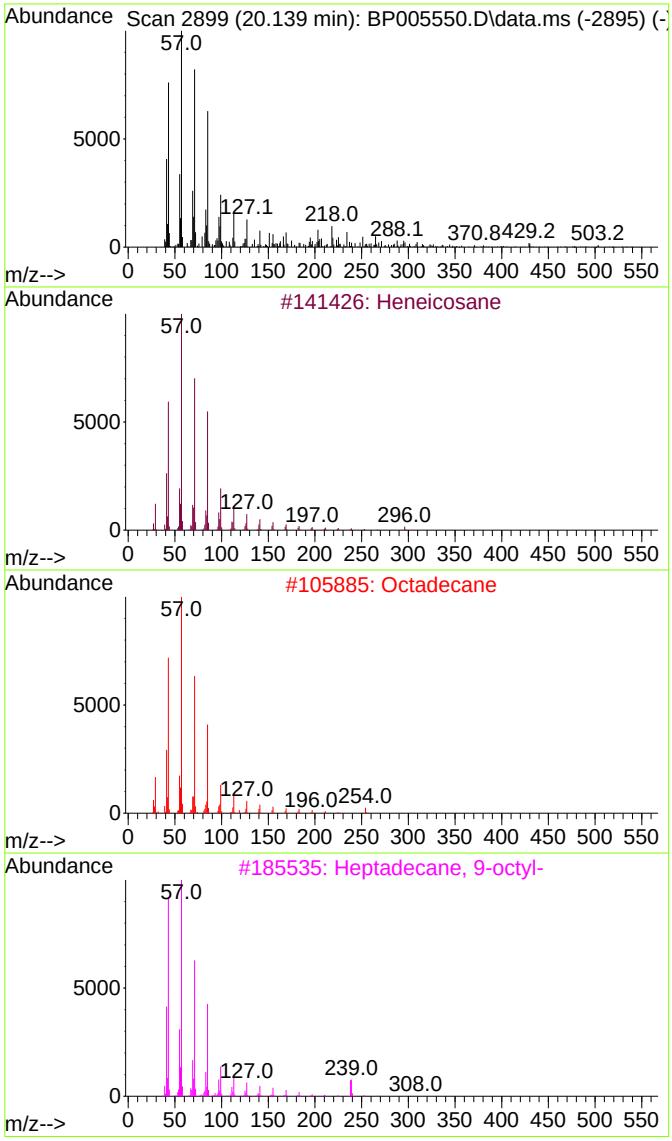
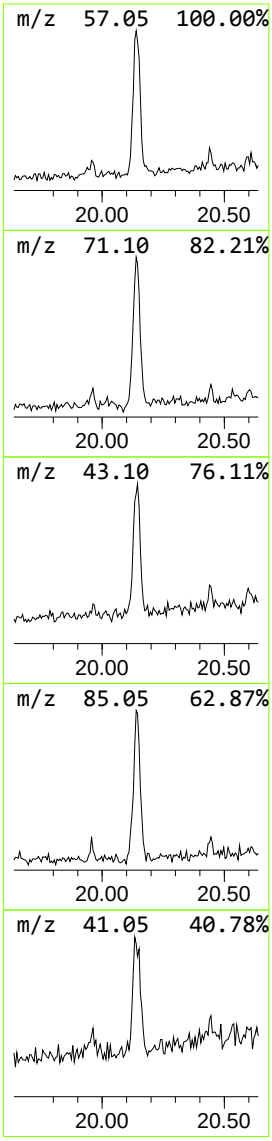
Peak Number 11 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.139	6.20 ng	131262	Chrysene-d12	21.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Octadecane	254	C18H38	000593-45-3	93
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	91
5	Nonadecane	268	C19H40	000629-92-5	91





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Data File : BP005550.D
Acq On : 14 May 2021 15:52
Operator : CG/JU
Sample : M2373-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
OR-02-051221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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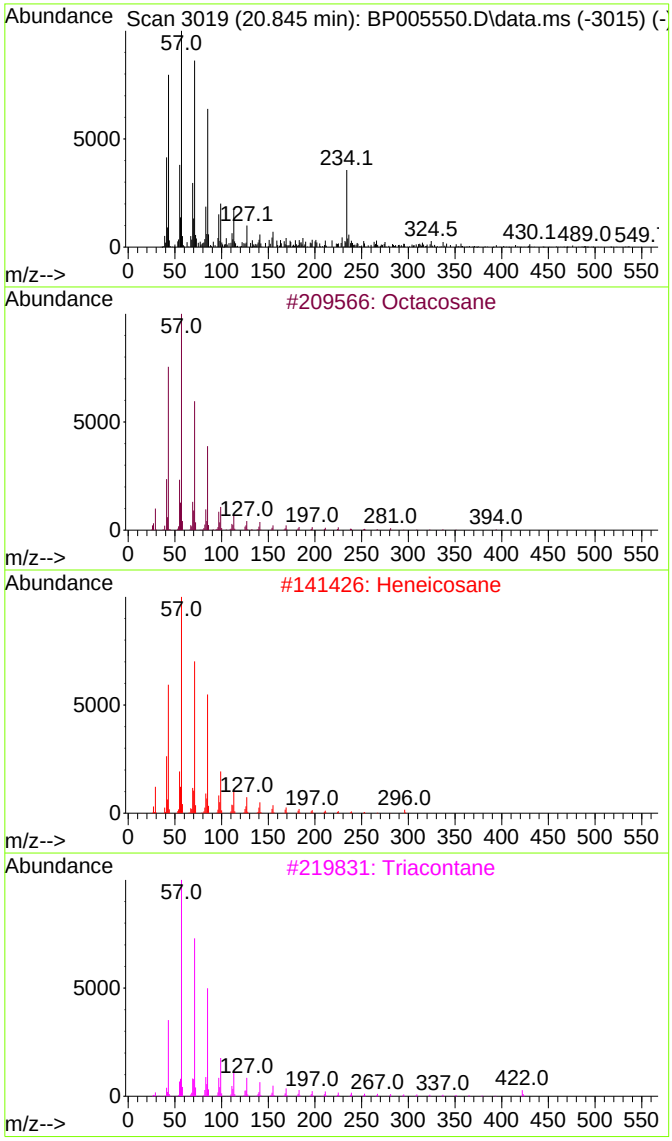
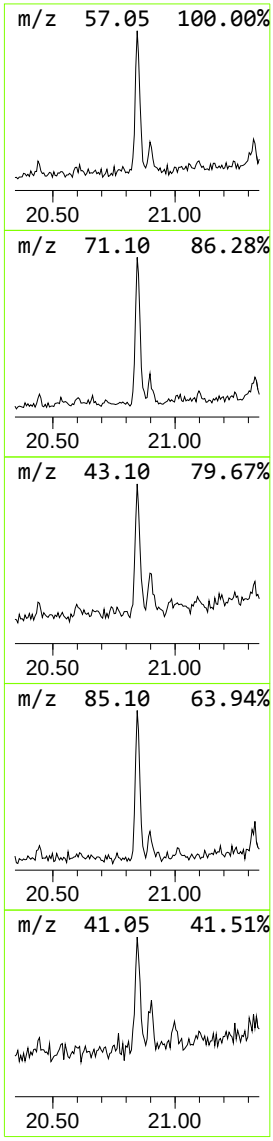
Peak Number 12 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.845	6.92 ng	146436	Chrysene-d12	21.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	96
2	Heneicosane	296	C21H44	000629-94-7	93
3	Triacontane	422	C30H62	000638-68-6	81
4	Pentatriacontane	493	C35H72	000630-07-9	76
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051421\
Data File : BP005550.D
Acq On : 14 May 2021 15:52
Operator : CG/JU
Sample : M2373-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
OR-02-051221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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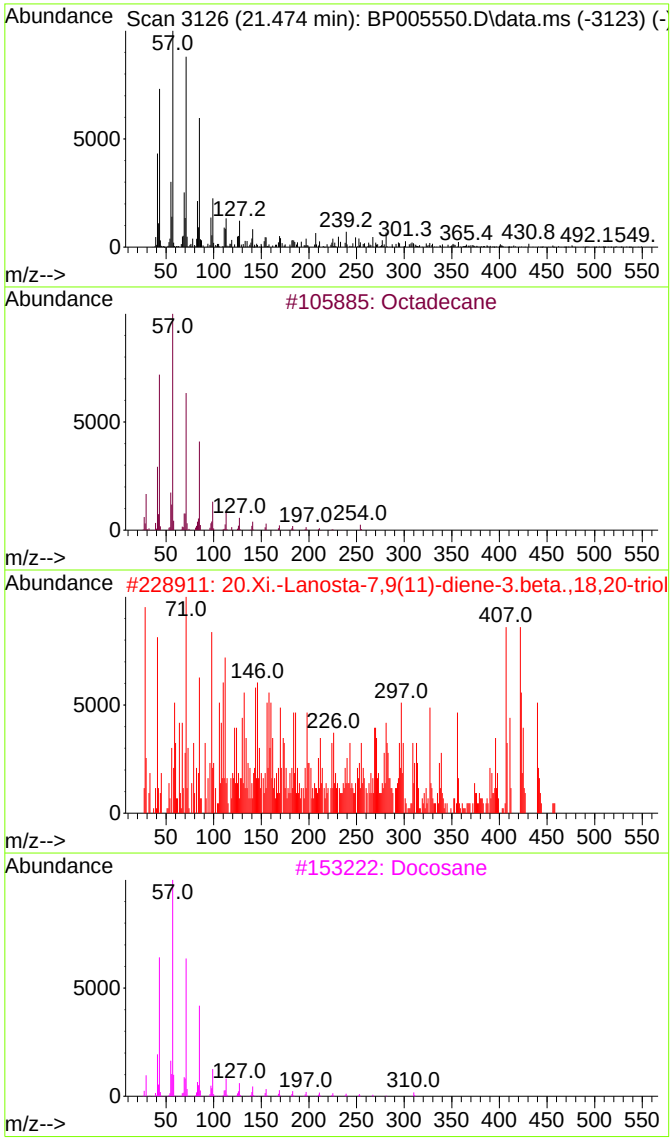
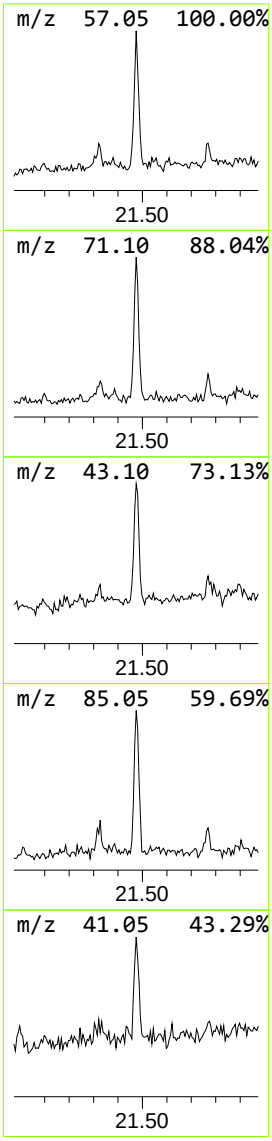
Peak Number 13 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.474	6.31 ng	133498	Chrysene-d12	21.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	97
2	20.Xi.-Lanosta-7,9(11)-diene-3.b...	458	C30H50O3	025116-58-9	95
3	Docosane	310	C22H46	000629-97-0	94
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	91
5	Heptadecane	240	C17H36	000629-78-7	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051421\
Data File : BP005550.D
Acq On : 14 May 2021 15:52
Operator : CG/JU
Sample : M2373-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : OR-02-051221

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown16.50	16.504	3.9	ng	45069	4	17.086	231213	20.0
3-Octanone, 2-m...	16.757	3.7	ng	42771	4	17.086	231213	20.0
Tetradecanoic acid	17.992	8.3	ng	95985	4	17.086	231213	20.0
Benzamide, N-pr...	18.121	56.4	ng	652432	4	17.086	231213	20.0
1,2-Propanedion...	18.274	83.5	ng	965772	4	17.086	231213	20.0
2,2'-(Ethane-1,...	18.410	163.2	ng	1886490	4	17.086	231213	20.0
Benzamide, N-ac...	18.557	10.5	ng	121723	4	17.086	231213	20.0
Phenanthrene, 2...	18.851	2.0	ng	23199	4	17.086	231213	20.0
Octadecanoic acid	19.227	2.1	ng	44463	5	21.186	423101	20.0
Tridecane, 3-me...	19.316	5.0	ng	104612	5	21.186	423101	20.0
Heneicosane	20.139	6.2	ng	131262	5	21.186	423101	20.0
Octacosane	20.845	6.9	ng	146436	5	21.186	423101	20.0
Octadecane	21.474	6.3	ng	133498	5	21.186	423101	20.0