LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP123021\
Data File : BP008608.D
Acq On : 30 Dec 2021 13:57
Operator : CG/JU
Sample : M5210-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R206

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-BP122821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008608.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.087	16	17	24	rVB	279402	267614	1.36%	0.183%
2	3.611	102	106	117	rVB	204817	296885	1.51%	0.203%
3	5.470	415	422	438	rVB	5944692	8791755	44.59%	6.018%
4	7.058	684	692	702	rBV	5282195	8855871	44.92%	6.062%
5	7.893	826	834	842	rBV	1575604	2517327	12.77%	1.723%
6	9.046	1022	1030	1043	rBV	3383936	5647717	28.65%	3.866%
7	9.922	1169	1179	1189	rBV	125801	327417	1.66%	0.224%
8	10.693	1299	1310	1317	rBV	1984906	3399104	17.24%	2.327%
9	13.152	1720	1728	1738	rVB	9287351	13456106	68.25%	9.210%
10	14.522	1952	1961	1967	rBV	2943072	4426360	22.45%	3.030%
11	14.587	1967	1972	1980	rVB	221723	349468	1.77%	0.239%
12	14.922	2019	2029	2030	rBV	156224	226948	1.15%	0.155%
13	14.940	2030	2032	2038	rVB	171855	230974	1.17%	0.158%
14	15.569	2134	2139	2152	rVB2	234871	377452	1.91%	0.258%
15	16.010	2207	2214	2223	rBV	6405347	9296551	47.15%	6.363%
16	16.363	2269	2274	2278	rBV	156914	234869	1.19%	0.161%
17	16.422	2278	2284	2289	rVV2	170653	338308	1.72%	0.232%
18	16.481	2289	2294	2298	rVB2	142266	211757	1.07%	0.145%
19	16.681	2323	2328	2334	rBV4	210287	352332	1.79%	0.241%
20	16.745	2335	2339	2343	rBV	158153	211901	1.07%	0.145%
21	17.269	2422	2428	2432	rBV	3416532	4908181	24.89%	3.360%
22	17.310	2432	2435	2442	rVB	973201	1432625	7.27%	0.981%
23	17.669	2492	2496	2501	rVB	145672	199463	1.01%	0.137%
24	17.951	2540	2544	2549	rBV	516185	621702	3.15%	0.426%
25	18.051	2556	2561	2567	rBV2	259496	506559	2.57%	0.347%
26	18.175	2573	2582	2603	rBV	8135359	13168804	66.79%	9.014%
27	18.322	2604	2607	2611	rVB2	163919	253665	1.29%	0.174%
28	19.081	2732	2736	2740	rVB2	902442	1010994	5.13%	0.692%
29	19.210	2755	2758	2762	rBV	209111	246516	1.25%	0.169%
30	19.281	2764	2770	2784	rBV2	2643498	5673490	28.78%	3.883%
31	19.410	2786	2792	2808	rVV	12352652	19715895	100.00%	13.495%
32	19.628	2825	2829	2838	rVB2	1237959	2092781	10.61%	1.432%
33	19.828	2858	2863	2872	rVB	13771348	16666685	84.53%	11.408%
34	20.110	2908	2911	2914	rVB2	244441	278865	1.41%	0.191%
35	20.445	2965	2968	2973	rBV4	217464	299151	1.52%	0.205%
36	21.004	3060	3063	3067	rBV	248790	282559	1.43%	0.193%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP123021\
Data File : BP008608.D
Acq On : 30 Dec 2021 13:57
Operator : CG/JU
Sample : M5210-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R206

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-BP122821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.069	3070	3074	3081	rVV2	1444492	1775127	9.00%	1.215%
38	21.351	3116	3122	3126	rBV	4800761	6849661	34.74%	4.688%
39	21.386	3126	3128	3136	rVB	574751	679805	3.45%	0.465%
40	23.057	3404	3412	3429	rVB2	570677	2264253	11.48%	1.550%
41	23.774	3527	3534	3541	rBV2	3601652	7354541	37.30%	5.034%

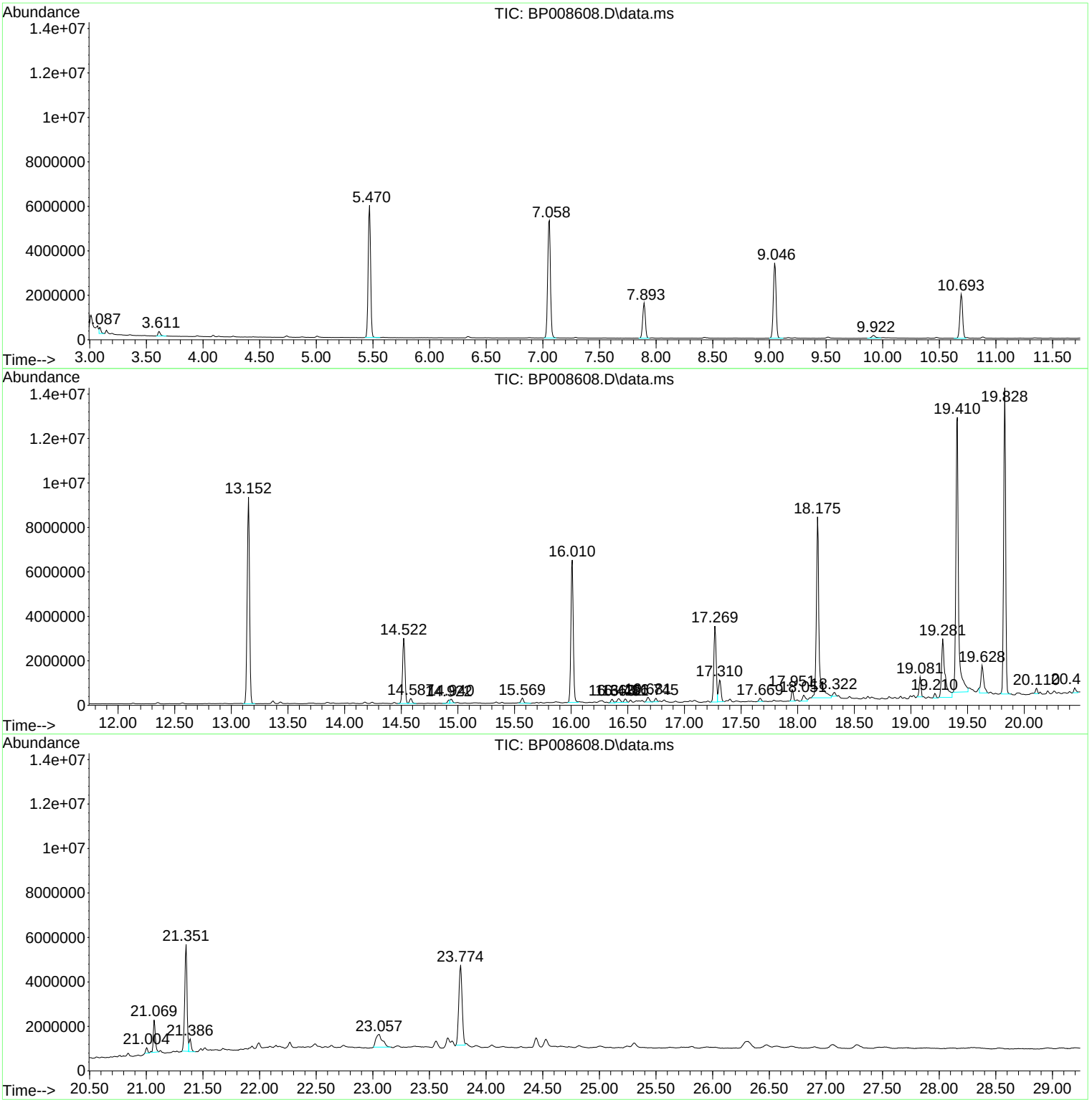
Sum of corrected areas: 146098038

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP123021\
Data File : BP008608.D
Acq On : 30 Dec 2021 13:57
Operator : CG/JU
Sample : M5210-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R206

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.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\BP123021\
Data File : BP008608.D
Acq On : 30 Dec 2021 13:57
Operator : CG/JU
Sample : M5210-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R206

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

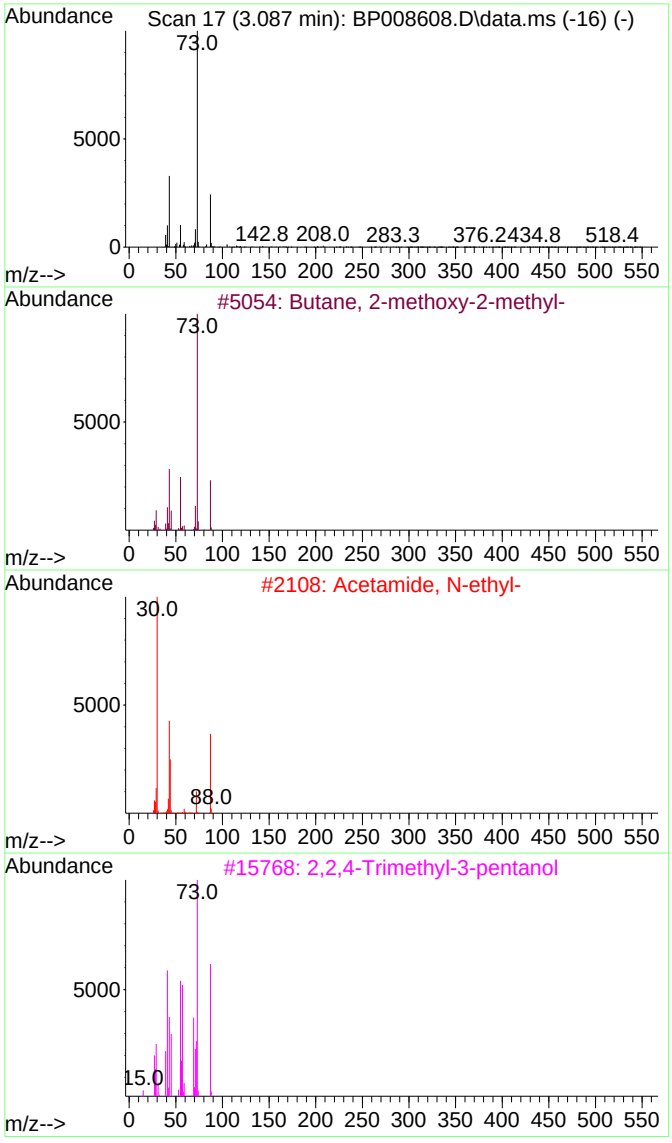
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

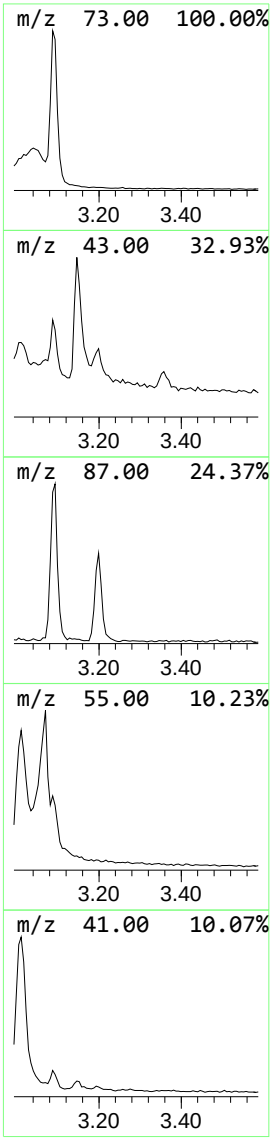
****

Peak Number 1 unknown3.087 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	2.13 ng	267614	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	39
2	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9
4	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP123021\
Data File : BP008608.D
Acq On : 30 Dec 2021 13:57
Operator : CG/JU
Sample : M5210-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R206

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

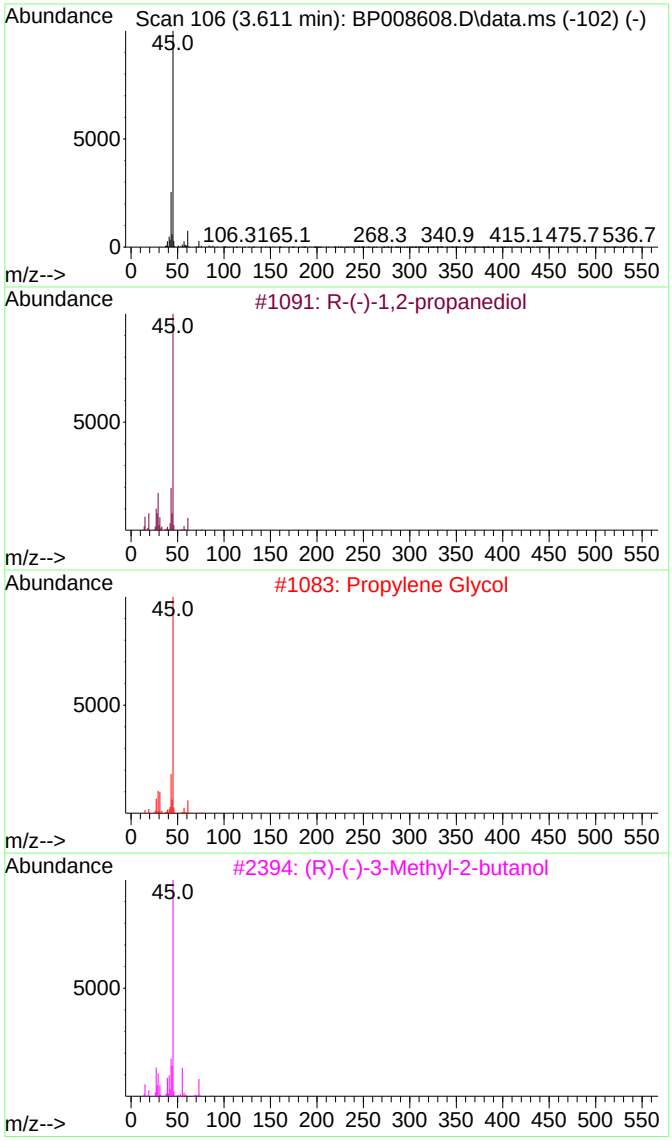
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

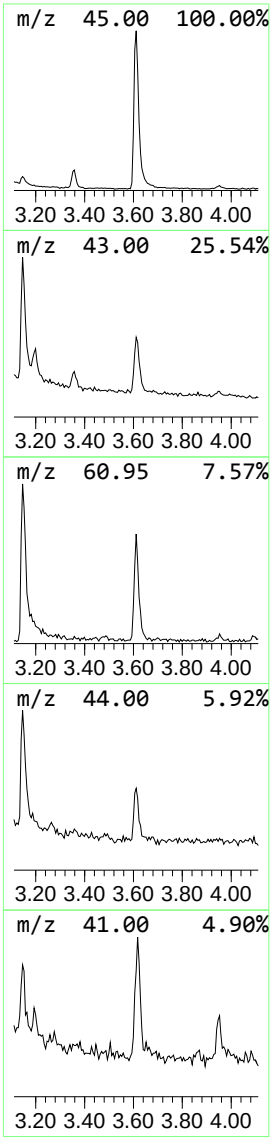
****

Peak Number 2 R-(-)-1,2-propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.611	2.36 ng	296885	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
2	Propylene Glycol	76	C3H8O2	000057-55-6	72
3	(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	56
4	2-Methoxyisopropyl cyanoacetate	157	C7H11NO3	032804-79-8	50
5	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP123021\
Data File : BP008608.D
Acq On : 30 Dec 2021 13:57
Operator : CG/JU
Sample : M5210-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R206

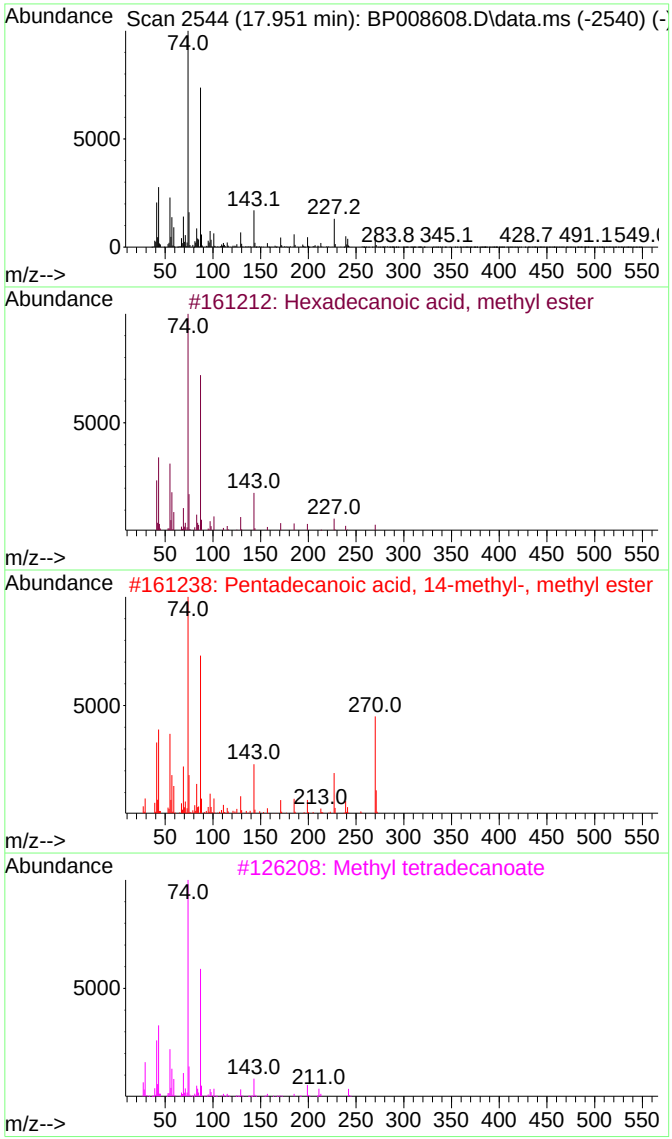
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

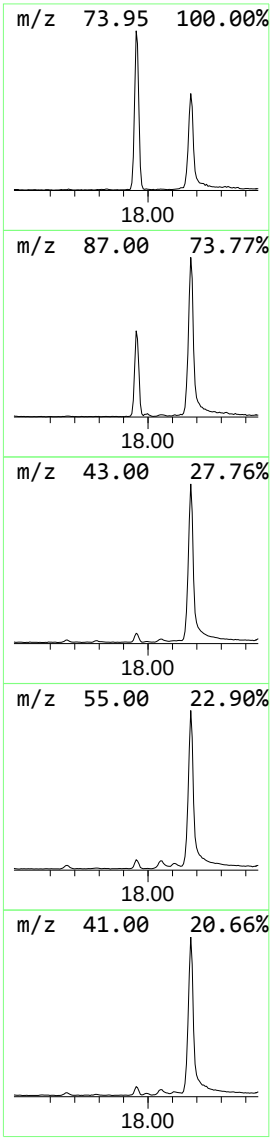
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.951	2.53 ng	621702	Phenanthrene-d10	17.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	83
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80
5	Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP123021\
Data File : BP008608.D
Acq On : 30 Dec 2021 13:57
Operator : CG/JU
Sample : M5210-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R206

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

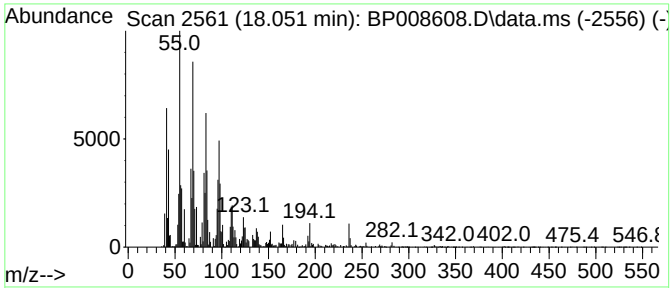
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

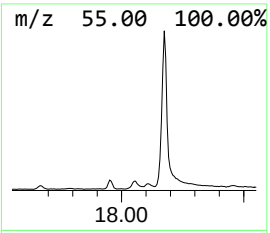
****

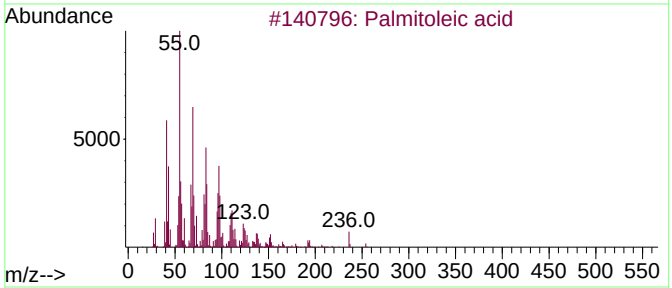
Peak Number 4 Palmitoleic acid Concentration Rank 8

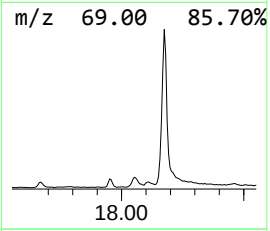
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.051	2.06 ng	506559	Phenanthrene-d10	17.269

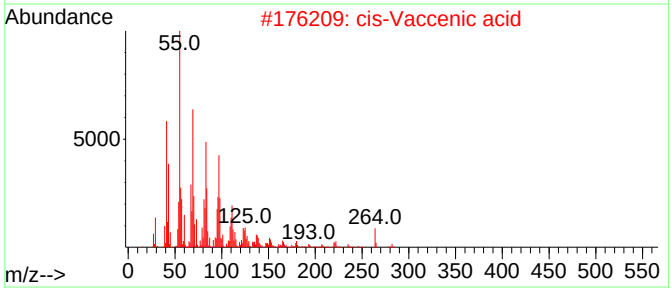
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Palmitoleic acid	254	C16H30O2	000373-49-9	99
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	98
3	6-Pentadecenoic acid, 13-methyl-...	254	C16H30O2	682751-34-4	95
4	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	93
5	Pyridine-3-carboxamide, oxime, N...	281	C13H10F3N3O	288246-53-7	93

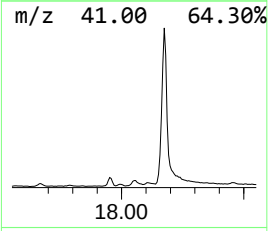


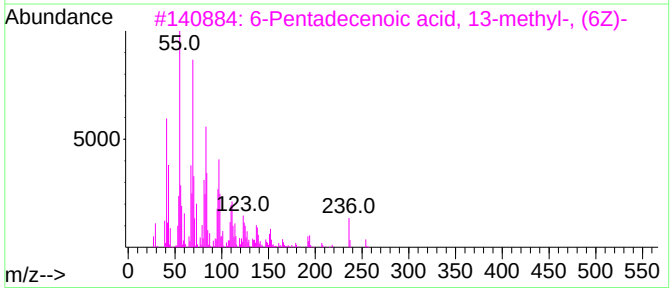


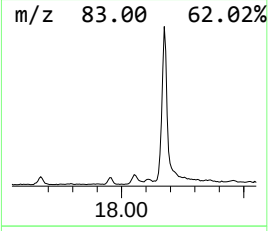


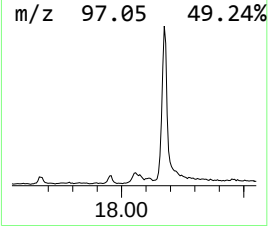












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP123021\
Data File : BP008608.D
Acq On : 30 Dec 2021 13:57
Operator : CG/JU
Sample : M5210-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R206

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

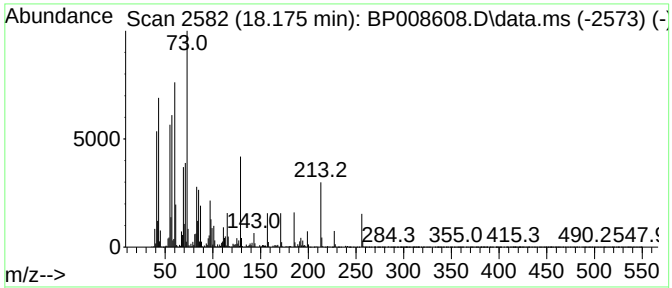
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

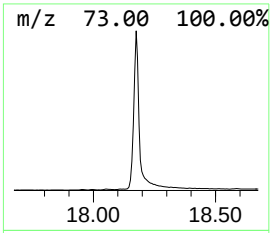
****

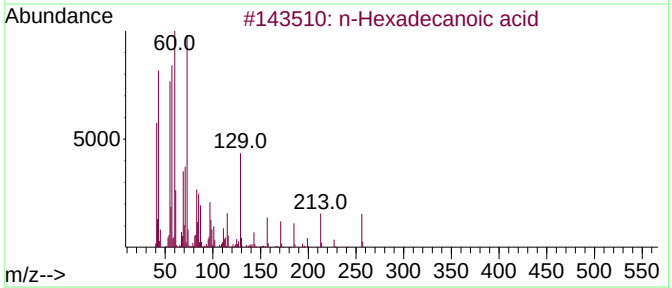
Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

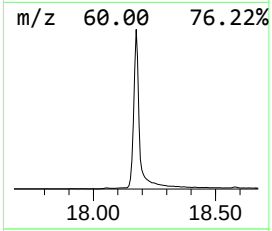
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.175	53.66 ng	13168800	Phenanthrene-d10	17.269

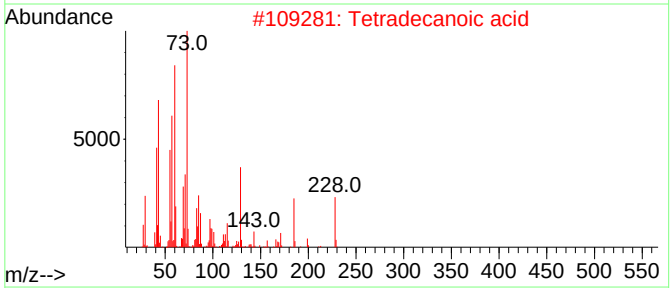
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Octadecanoic acid	284	C18H36O2	000057-11-4	90
5	Undecanoic acid	186	C11H22O2	000112-37-8	83

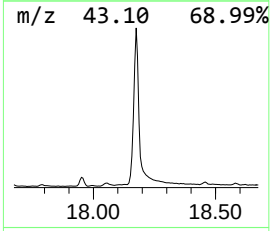


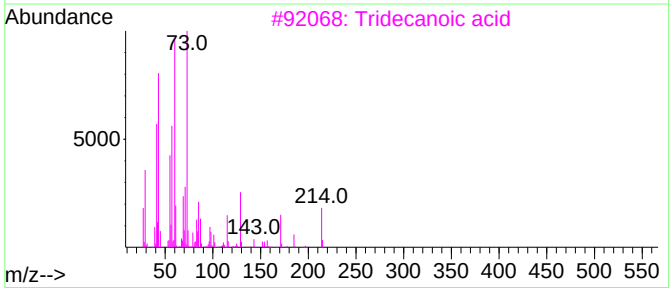


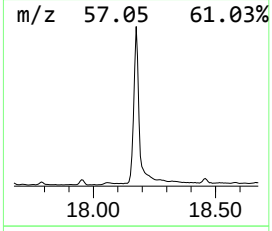


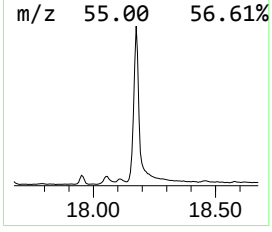












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP123021\
Data File : BP008608.D
Acq On : 30 Dec 2021 13:57
Operator : CG/JU
Sample : M5210-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R206

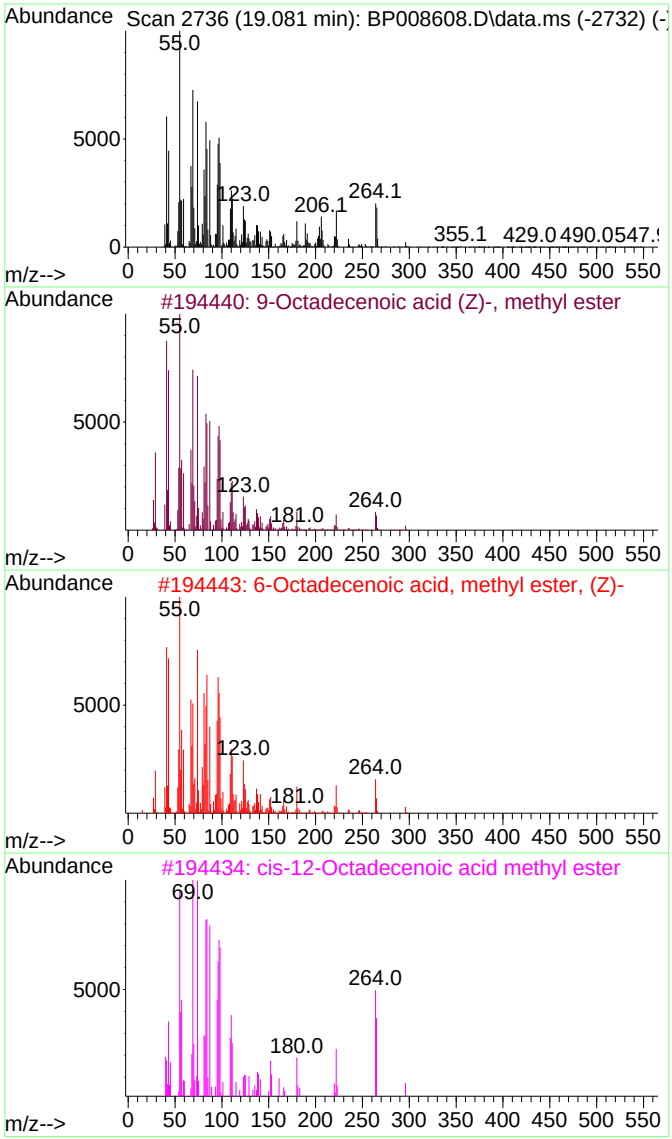
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

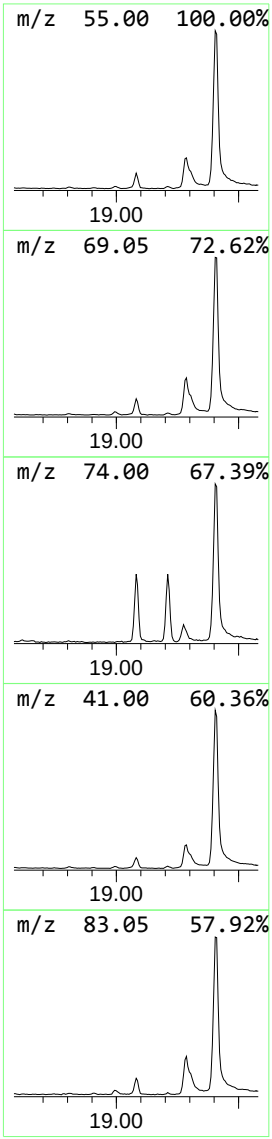
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.081	4.12 ng	1010990	Phenanthrene-d10	17.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	99
3	cis-12-Octadecenoic acid methyl ...	296	C19H36O2	1000427-68-4	99
4	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
5	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99





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Data File : BP008608.D
Acq On : 30 Dec 2021 13:57
Operator : CG/JU
Sample : M5210-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R206

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.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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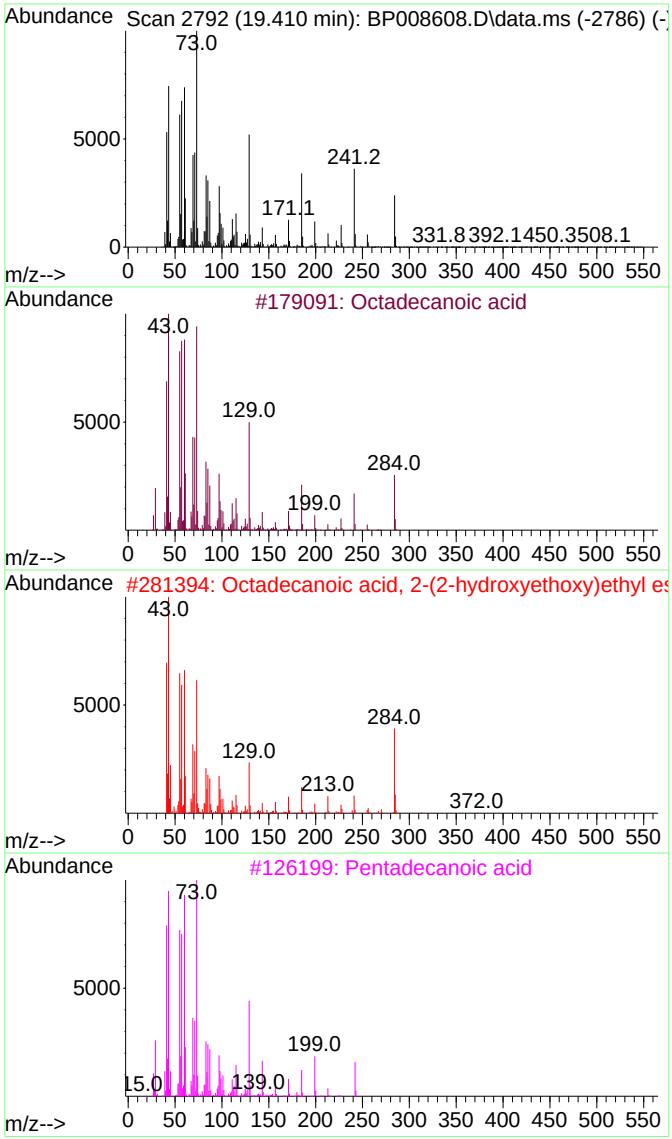
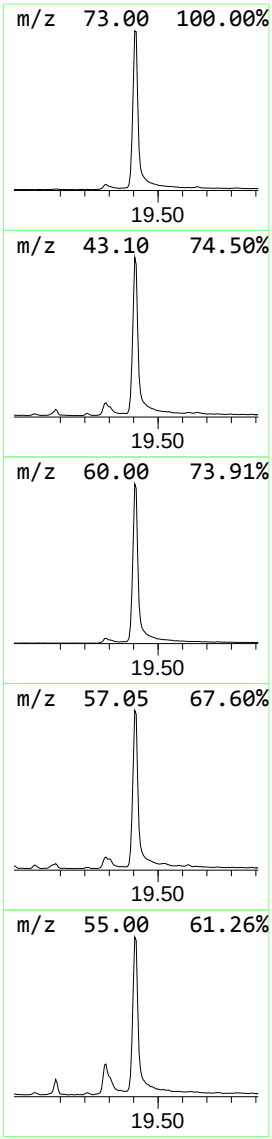
Peak Number 7 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.410	57.57 ng	19715900	Chrysene-d12	21.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP123021\
Data File : BP008608.D
Acq On : 30 Dec 2021 13:57
Operator : CG/JU
Sample : M5210-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R206

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.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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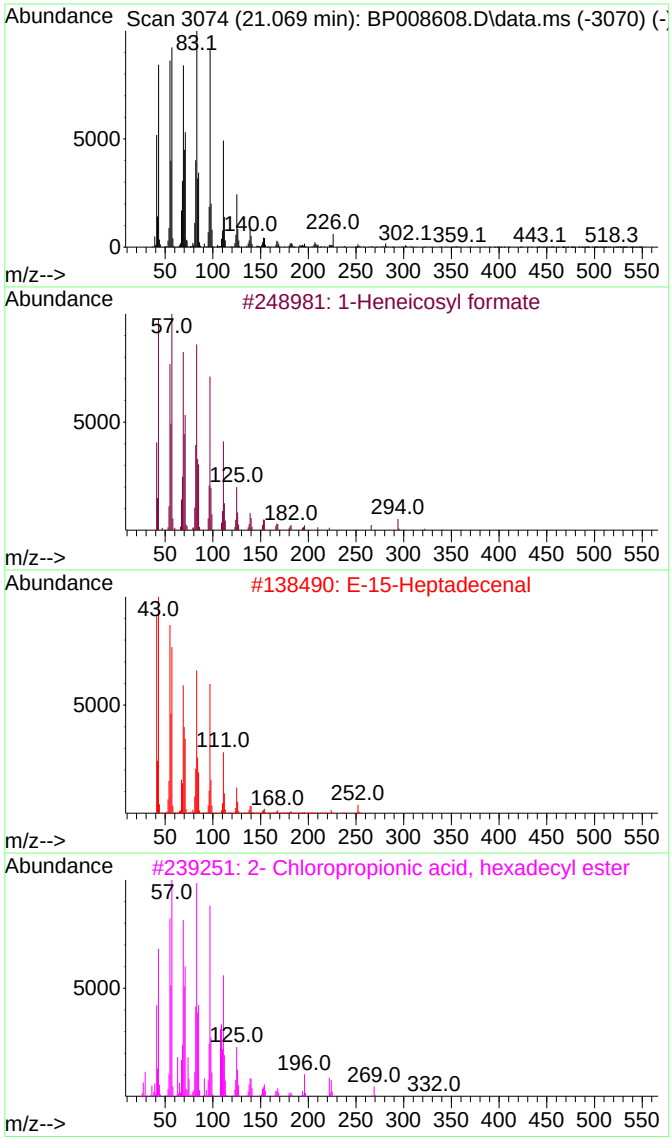
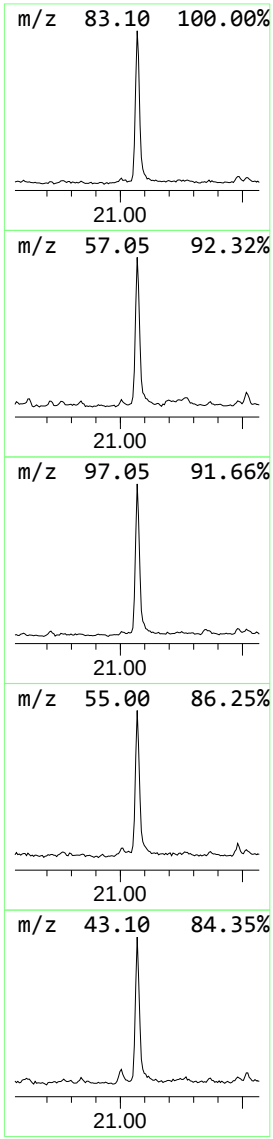
Peak Number 8 1-Heneicosyl formate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.069	5.18 ng	1775130	Chrysene-d12	21.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	96
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	96
3	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP123021\
Data File : BP008608.D
Acq On : 30 Dec 2021 13:57
Operator : CG/JU
Sample : M5210-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R206

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP122821.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
unknown3.087	3.087	2.1	ng	267614	1	7.893	2517330	20.0
R-(-)-1,2-propa...	3.611	2.4	ng	296885	1	7.893	2517330	20.0
Hexadecanoic ac...	17.951	2.5	ng	621702	4	17.269	4908180	20.0
Palmitoleic acid	18.051	2.1	ng	506559	4	17.269	4908180	20.0
n-Hexadecanoic ...	18.175	53.7	ng	13168800	4	17.269	4908180	20.0
9-Octadecenoic ...	19.081	4.1	ng	1010990	4	17.269	4908180	20.0
Octadecanoic acid	19.410	57.6	ng	19715900	5	21.351	6849660	20.0
1-Heneicosyl fo...	21.069	5.2	ng	1775130	5	21.351	6849660	20.0