LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002330.D
Acq On : 29 May 2020 23:43
Operator : CG/JU
Sample : L2745-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM80-COMP-2020-0-6

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\8270-BP052720.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.999	15	19	28	rVB	95755	137602	1.06%	0.114%
2	4.552	273	283	314	rBV	110415	762602	5.89%	0.630%
3	5.222	391	397	410	rBV	4431415	6743675	52.11%	5.573%
4	6.799	654	665	678	rBV	4717324	7708282	59.56%	6.370%
5	7.216	731	736	742	rBV	93645	142946	1.10%	0.118%
6	7.605	793	802	812	rBV	1224824	1927781	14.90%	1.593%
7	7.928	848	857	866	rBV	3983467	6626731	51.21%	5.476%
8	8.752	986	997	1012	rBV	3251868	5390810	41.66%	4.455%
9	10.381	1266	1274	1288	rVB	1655721	2772006	21.42%	2.291%
10	12.869	1690	1697	1715	rBV	7008906	11166438	86.29%	9.228%
11	13.169	1741	1748	1755	rBV2	126428	212027	1.64%	0.175%
12	13.716	1834	1841	1852	rBV	715257	1136526	8.78%	0.939%
13	14.251	1926	1932	1939	rBV2	2471617	3613380	27.92%	2.986%
14	15.751	2176	2187	2195	rBV	5063377	7738177	59.79%	6.395%
15	16.404	2289	2298	2303	rBV3	223806	405277	3.13%	0.335%
16	16.945	2386	2390	2395	rBV	175662	272259	2.10%	0.225%
17	17.010	2395	2401	2405	rVV	2972766	4224977	32.65%	3.492%
18	17.051	2405	2408	2413	rVV	548325	738603	5.71%	0.610%
19	17.104	2413	2417	2420	rVV	130229	186591	1.44%	0.154%
20	17.139	2420	2423	2429	rVB	231632	318184	2.46%	0.263%
21	17.410	2465	2469	2477	rBV2	201526	310164	2.40%	0.256%
22	17.580	2495	2498	2507	rVB2	87784	138010	1.07%	0.114%
23	17.822	2533	2539	2544	rBV	165250	321926	2.49%	0.266%
24	17.880	2545	2549	2554	rVV2	277645	397642	3.07%	0.329%
25	17.945	2554	2560	2567	rVV2	991465	1446475	11.18%	1.195%
26	18.075	2578	2582	2586	rVB2	100003	135084	1.04%	0.112%
27	18.233	2605	2609	2620	rVB2	103670	170642	1.32%	0.141%
28	18.904	2719	2723	2726	rBV2	241650	354484	2.74%	0.293%
29	19.004	2735	2740	2743	rBV	2889618	3468342	26.80%	2.866%
30	19.033	2743	2745	2749	rVB	984136	1019318	7.88%	0.842%
31	19.180	2767	2770	2775	rBV	149247	205146	1.59%	0.170%
32	19.380	2797	2804	2808	rBV	831760	1335985	10.32%	1.104%
33	19.598	2836	2841	2850	rVB	9608152	12941230	100.00%	10.695%
34	20.245	2947	2951	2954	rBV	343070	378625	2.93%	0.313%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002330.D
Acq On : 29 May 2020 23:43
Operator : CG/JU
Sample : L2745-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM80-COMP-2020-0-6

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\8270-BP052720.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	20.833	3048	3051	3052	rBV	438450	422148	3.26%	0.349%
36	20.857	3052	3055	3065	rVB2	1498938	2035542	15.73%	1.682%
37	21.110	3092	3098	3102	rBV3	3302048	4637770	35.84%	3.833%
38	21.145	3102	3104	3111	rVB	433373	542601	4.19%	0.448%
39	21.298	3127	3130	3134	rVB3	284694	340889	2.63%	0.282%
40	21.739	3201	3205	3213	rVB	1031390	1504139	11.62%	1.243%
41	22.416	3316	3320	3328	rVB	830311	1119877	8.65%	0.925%
42	22.704	3364	3369	3372	rBV	1554411	2326654	17.98%	1.923%
43	22.733	3372	3374	3386	rVB	1723010	2586964	19.99%	2.138%
44	23.321	3469	3474	3489	rVB	2148507	4071669	31.46%	3.365%
45	23.574	3513	3517	3525	rVB	578339	1085655	8.39%	0.897%
46	23.927	3570	3577	3583	rBV	4077224	8042667	62.15%	6.647%
47	23.998	3584	3589	3597	rVB	1150502	2178093	16.83%	1.800%
48	25.551	3847	3853	3865	rVB2	869033	2512224	19.41%	2.076%
49	26.386	3989	3995	4015	rVB3	885307	2748715	21.24%	2.272%

Sum of corrected areas: 121003554

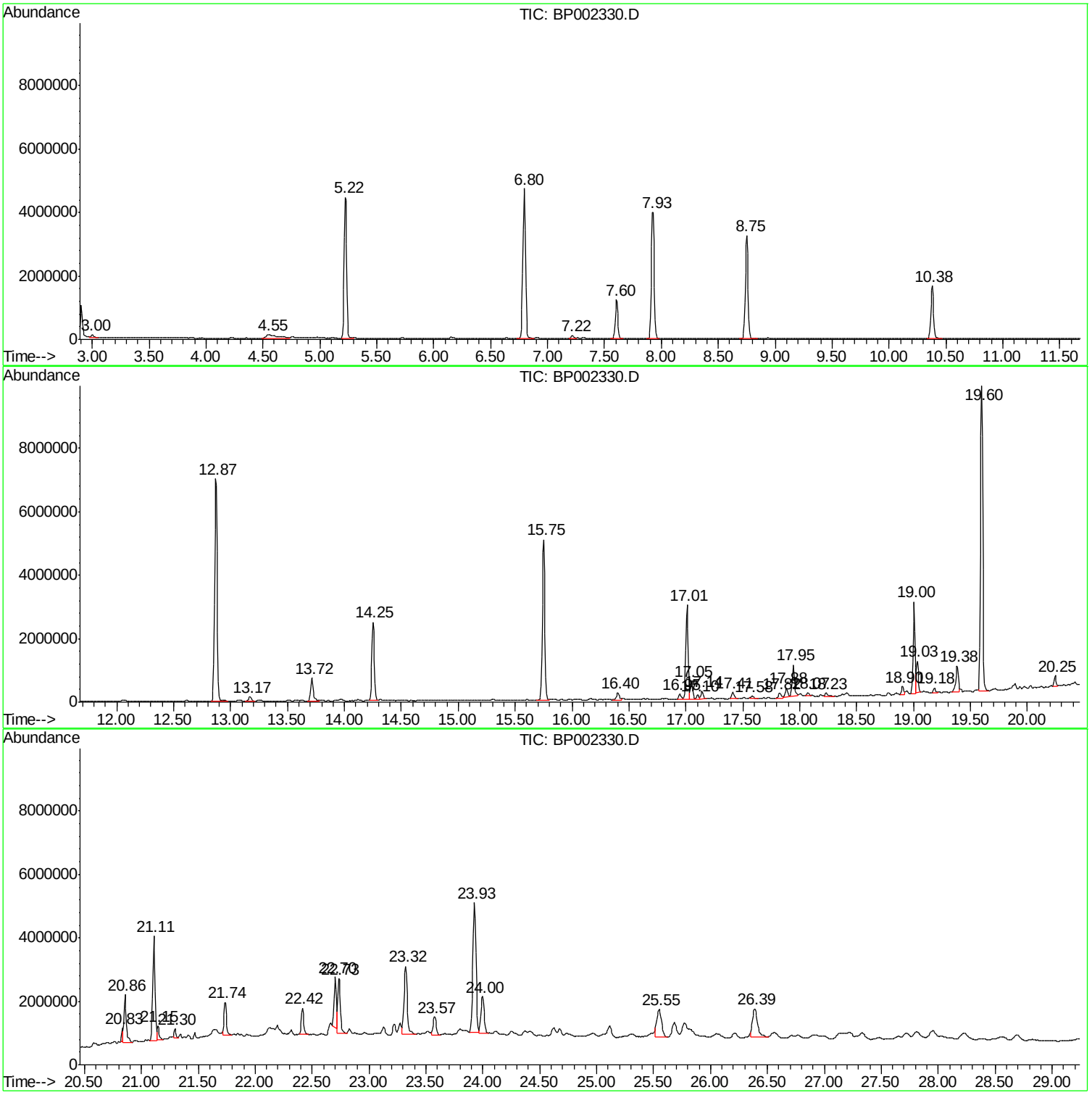
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002330.D
Acq On : 29 May 2020 23:43
Operator : CG/JU
Sample : L2745-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
NM80-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002330.D
Acq On : 29 May 2020 23:43
Operator : CG/JU
Sample : L2745-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM80-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.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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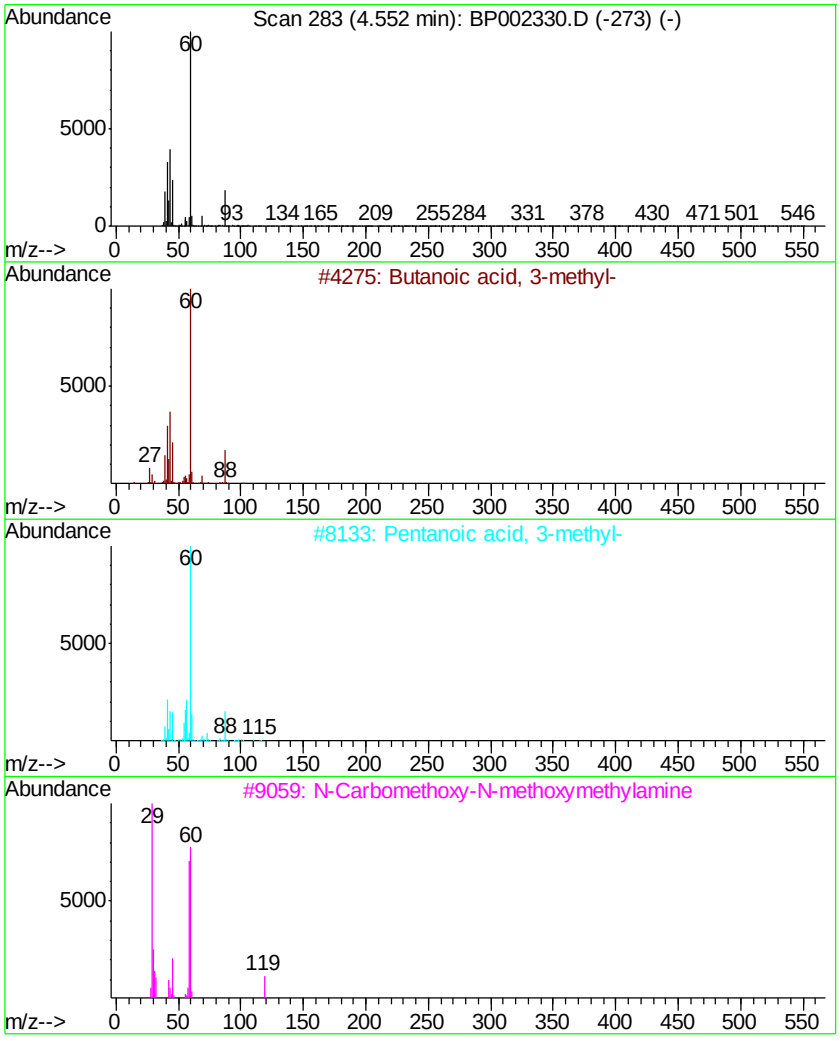
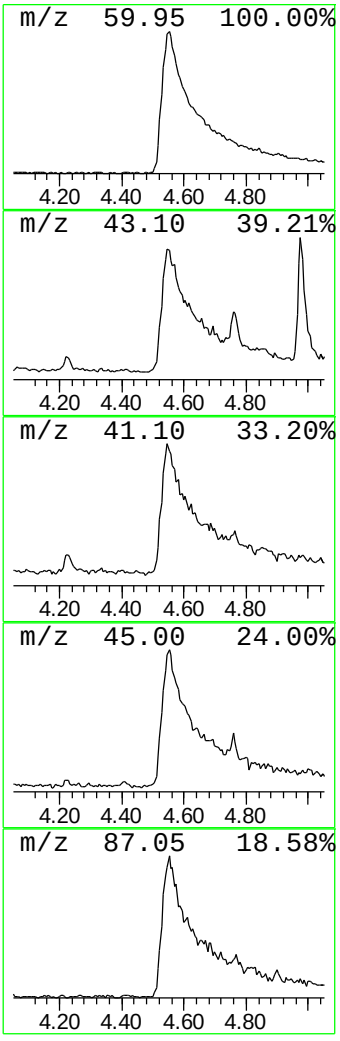
Peak Number 1 Butanoic acid, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	7.91 ng	762602	1,4-Dichlorobenzene-d4	7.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	90
2	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	72
3	N-Carbomethoxy-N-methoxymethylamine	119	C4H9NO3	153654-07-0	50
4	Pentanoic acid	102	C5H10O2	000109-52-4	38
5	Formic acid hydrazide	60	CH4N2O	000624-84-0	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002330.D
Acq On : 29 May 2020 23:43
Operator : CG/JU
Sample : L2745-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM80-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.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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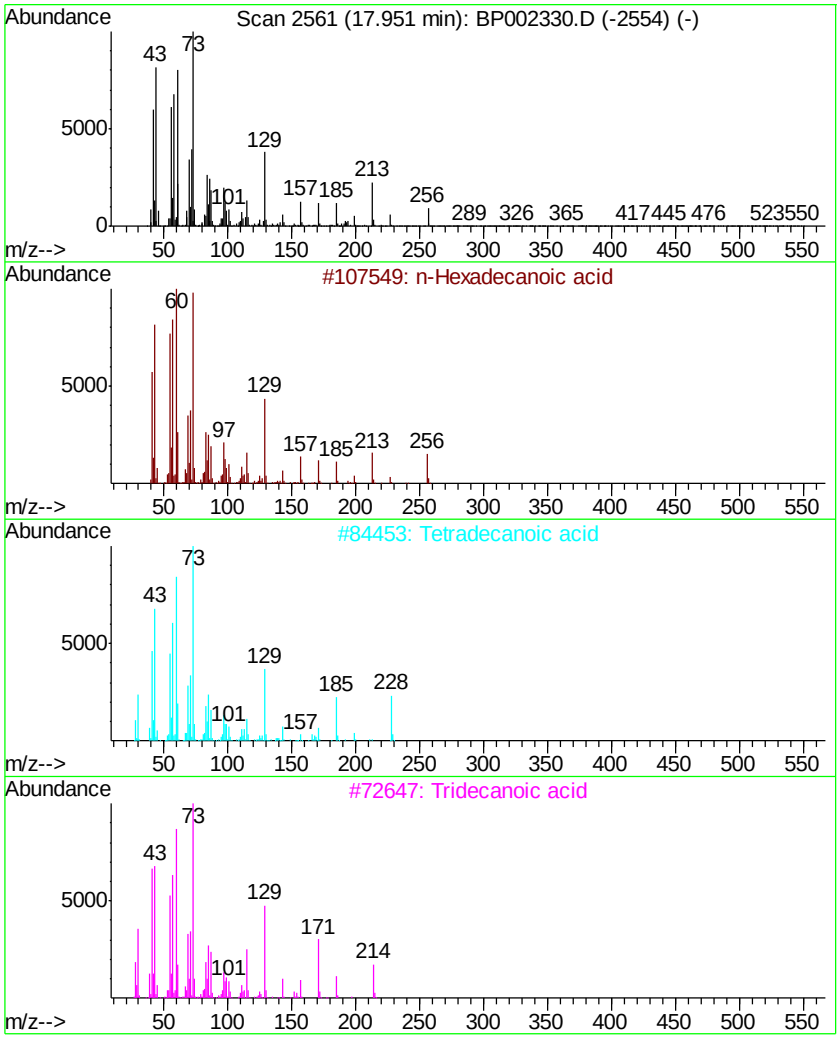
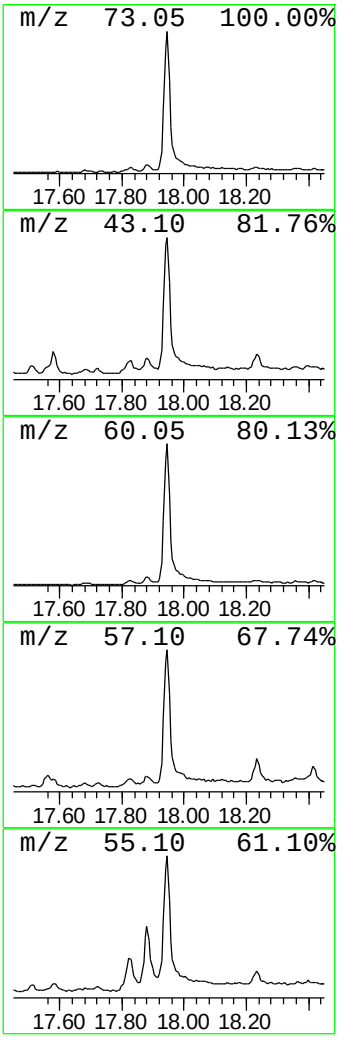
Peak Number 3 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.95	6.85 ng	1446480	Phenanthrene-d10	17.01

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	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002330.D
Acq On : 29 May 2020 23:43
Operator : CG/JU
Sample : L2745-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM80-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.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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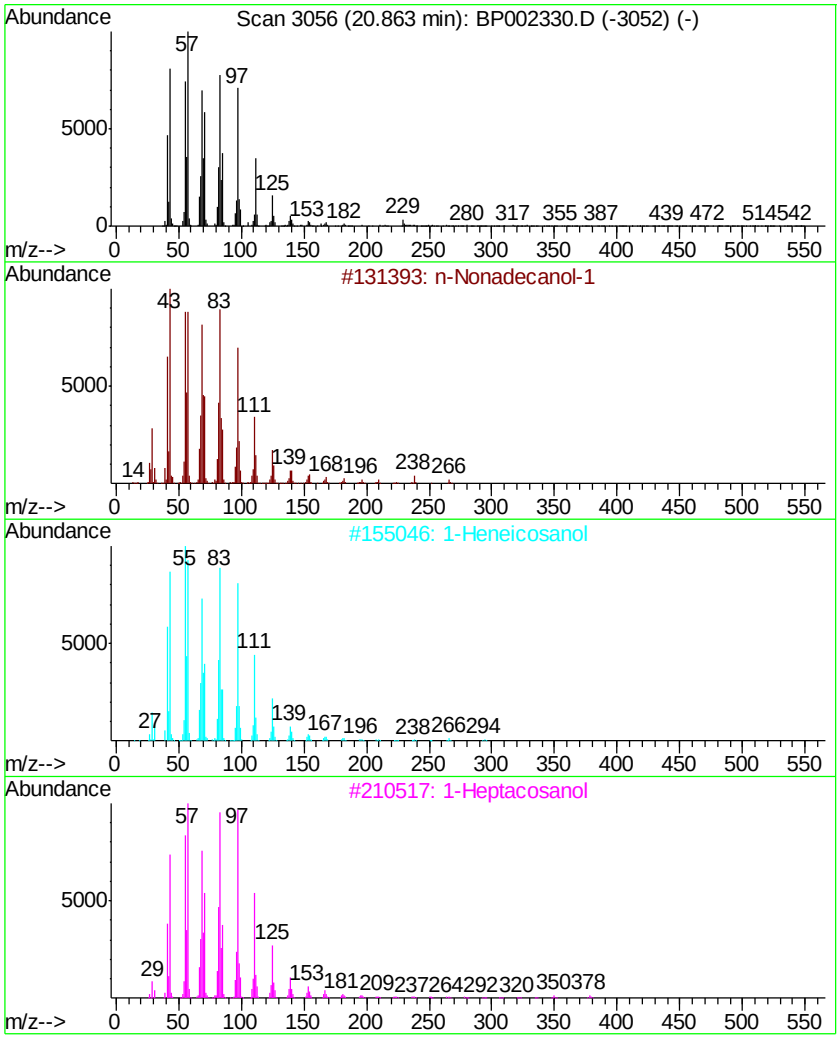
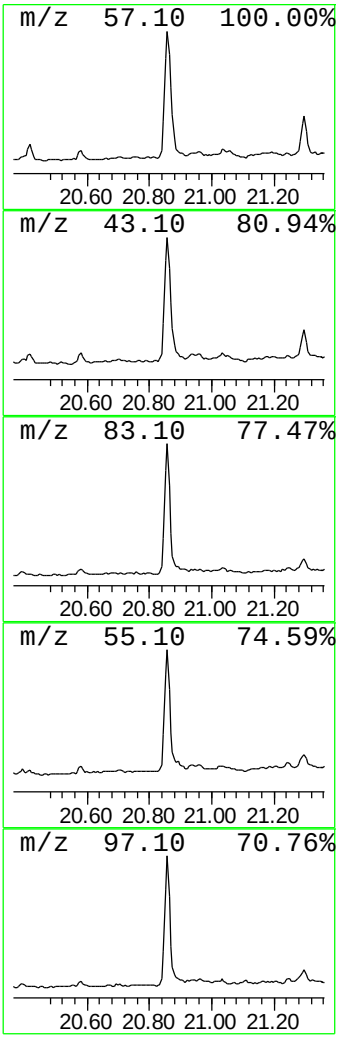
Peak Number 4 n-Nonadecanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	8.78 ng	2035540	Chrysene-d12	21.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	1-Heptacosanol	396	C27H56O	002004-39-9	94
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002330.D
Acq On : 29 May 2020 23:43
Operator : CG/JU
Sample : L2745-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM80-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.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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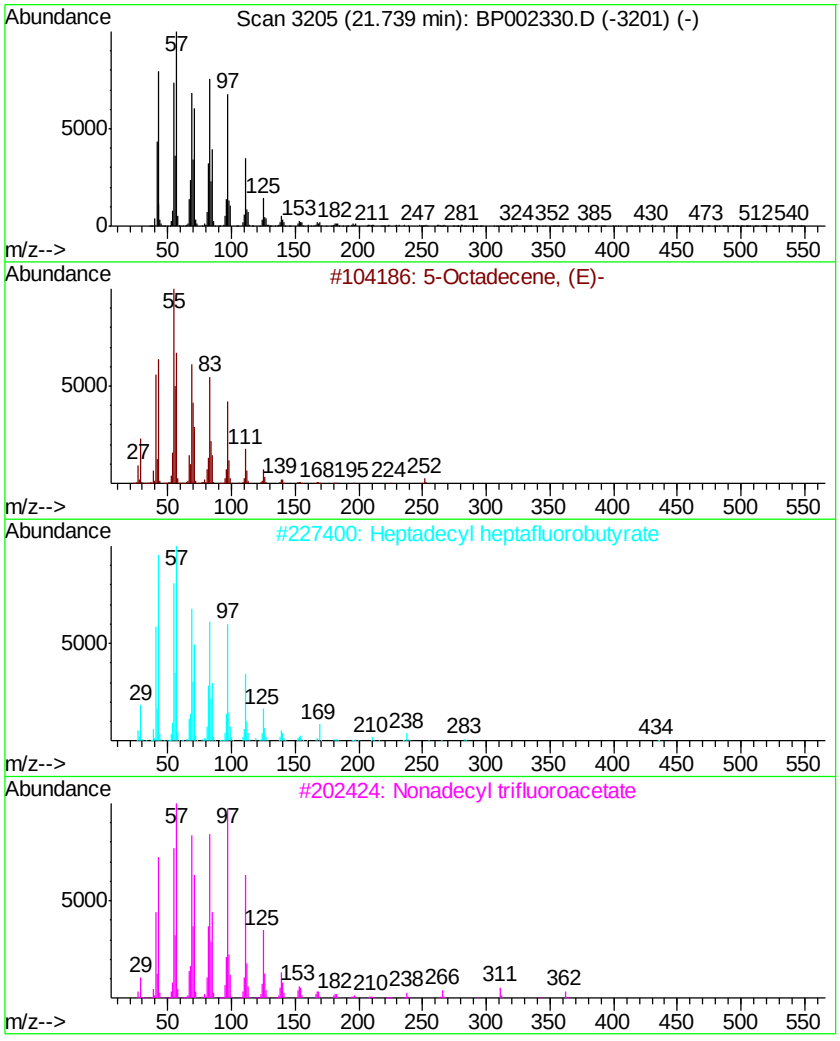
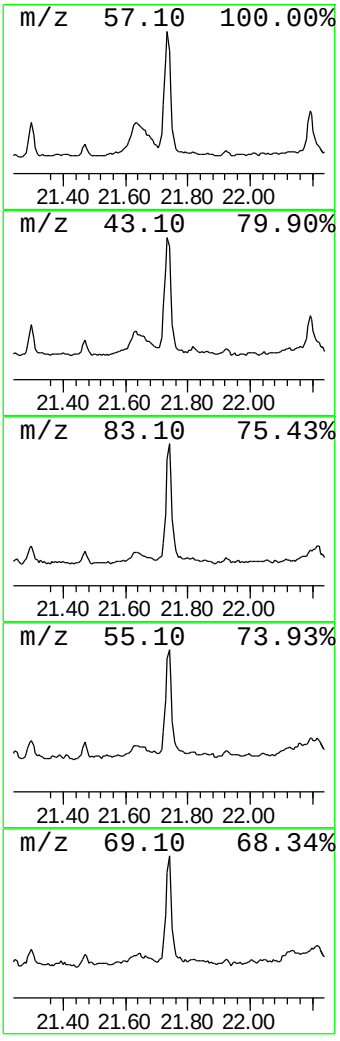
Peak Number 5 5-Octadecene, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.74	6.49 ng	1504140	Chrysene-d12	21.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	93
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	90
4	1-Heneicosanol	312	C21H44O	015594-90-8	89
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002330.D
Acq On : 29 May 2020 23:43
Operator : CG/JU
Sample : L2745-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM80-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.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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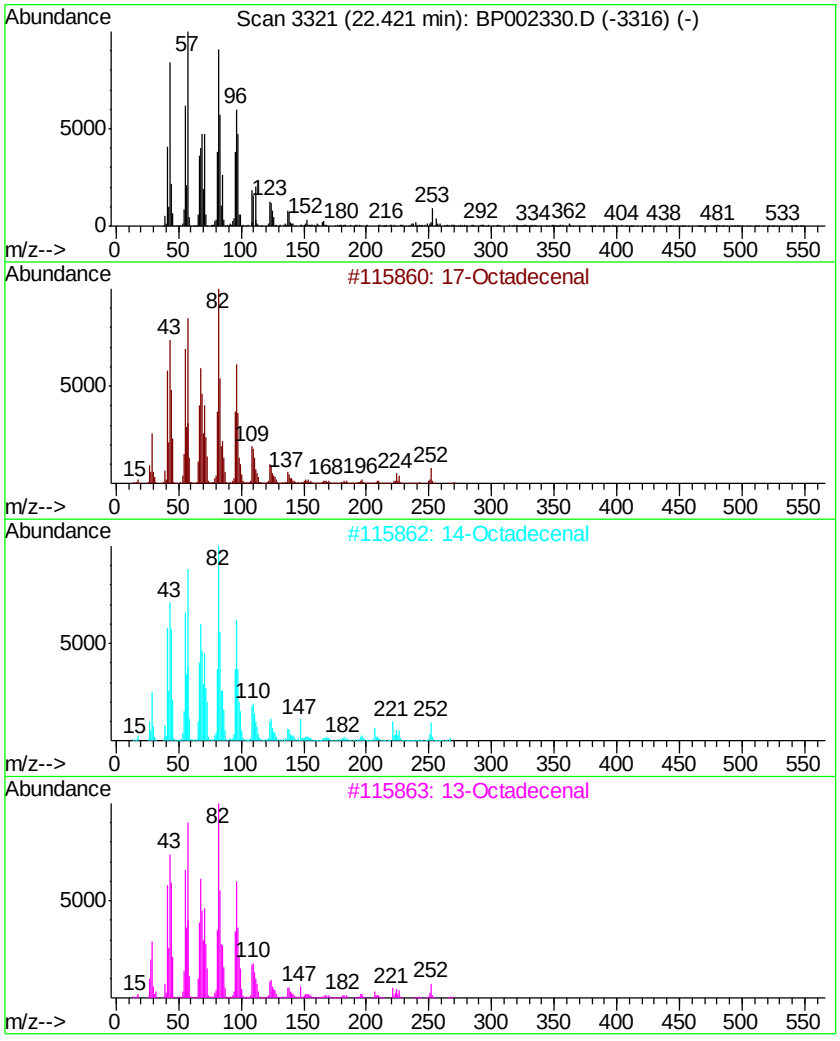
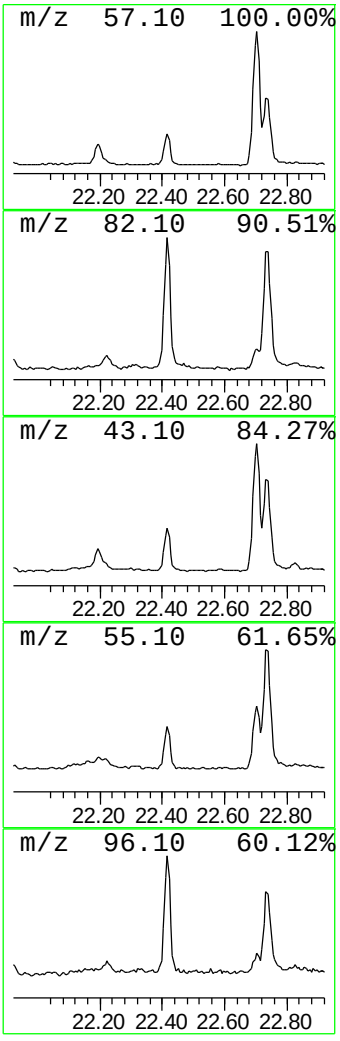
Peak Number 6 17-Octadecenal Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.42	5.50 ng	1119880	Perylene-d12	23.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Octadecenal	266	C18H34O	056554-86-0	93
2	14-Octadecenal	266	C18H34O	056554-89-3	91
3	13-Octadecenal	266	C18H34O	056554-90-6	91
4	16-Octadecenal	266	C18H34O	056554-87-1	91
5	Octadecanal	268	C18H36O	000638-66-4	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002330.D
Acq On : 29 May 2020 23:43
Operator : CG/JU
Sample : L2745-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM80-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.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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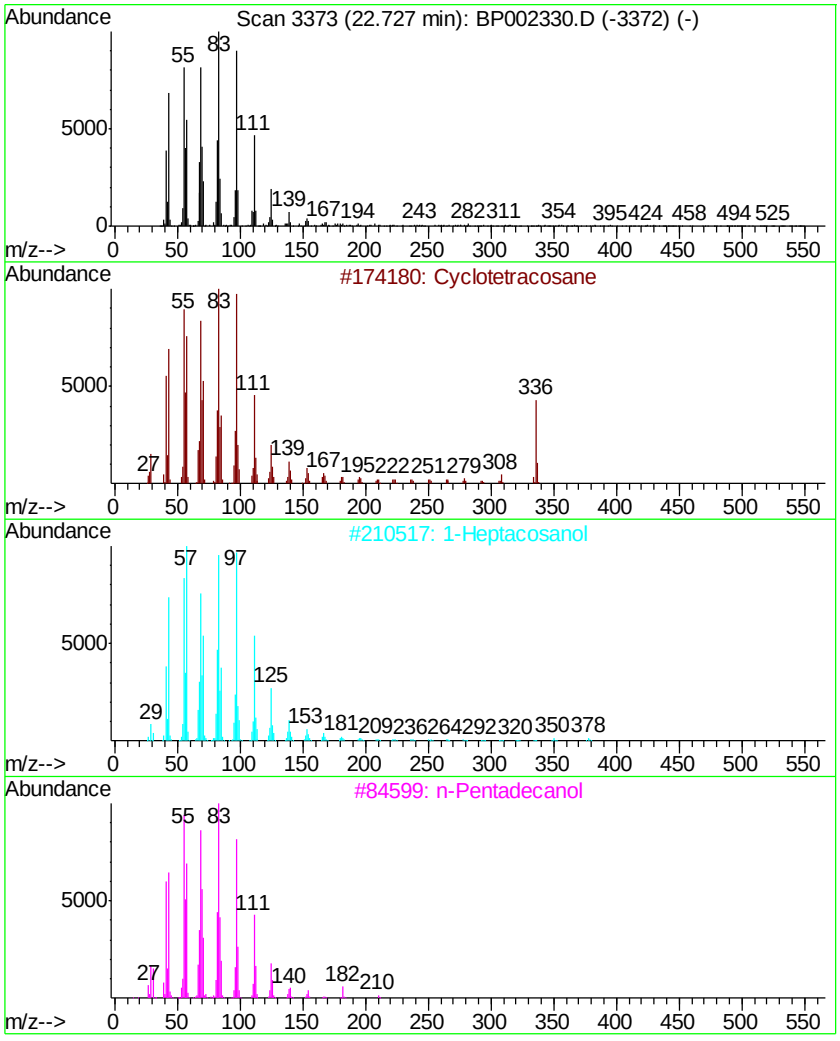
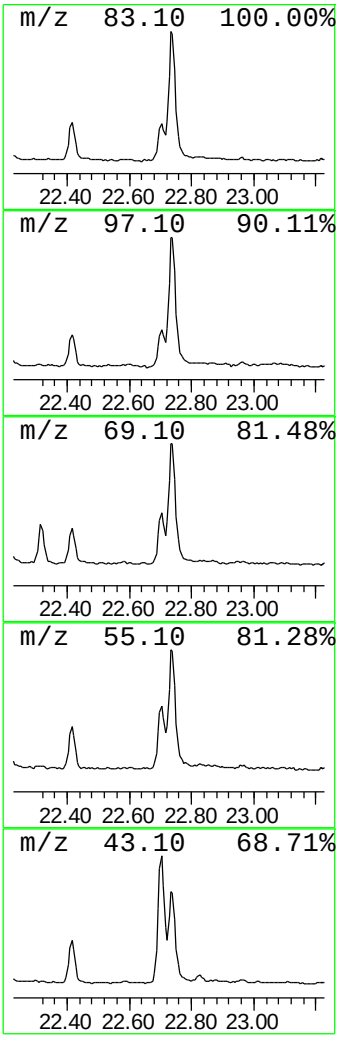
Peak Number 7 Cyclotetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.73	12.71 ng	2586960	Perylene-d12	23.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	91
2	1-Heptacosanol	396	C27H56O	002004-39-9	90
3	n-Pentadecanol	228	C15H32O	000629-76-5	87
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	76
5	1-Docosene	308	C22H44	001599-67-3	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002330.D
Acq On : 29 May 2020 23:43
Operator : CG/JU
Sample : L2745-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM80-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.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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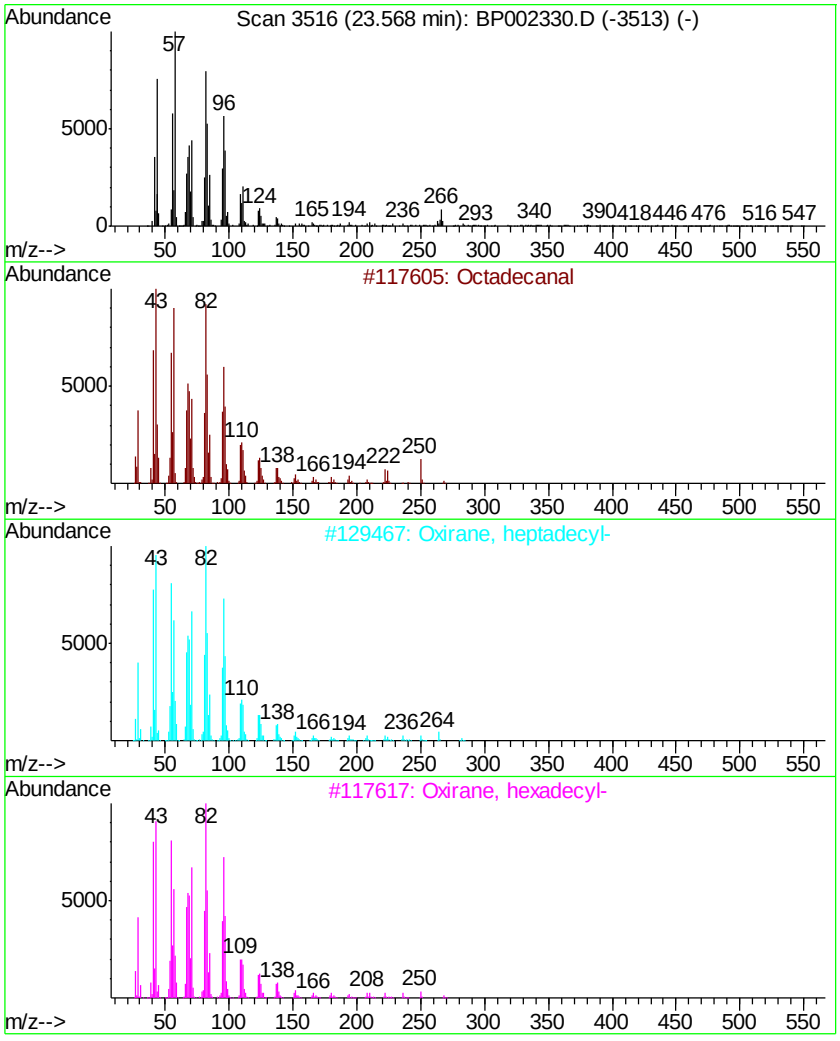
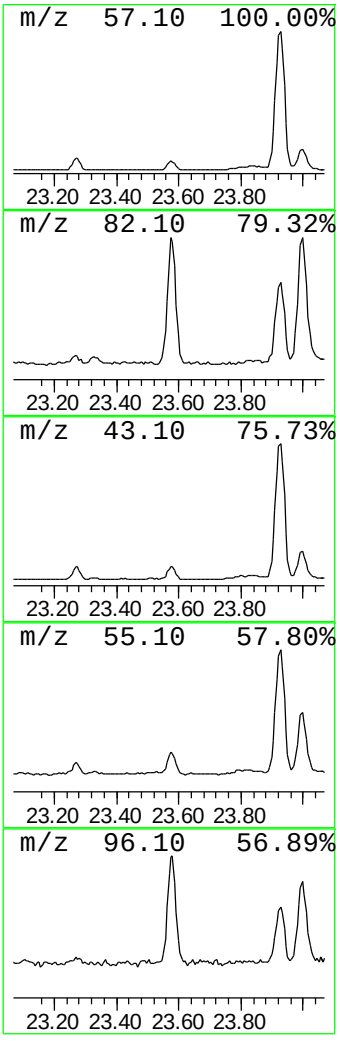
Peak Number 8 Octadecanal Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.57	5.33 ng	1085660	Perylene-d12	23.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
4	Tetradecanal	212	C14H28O	000124-25-4	87
5	Triacontyl acetate	480	C32H64O2	041755-58-2	74





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002330.D
Acq On : 29 May 2020 23:43
Operator : CG/JU
Sample : L2745-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM80-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.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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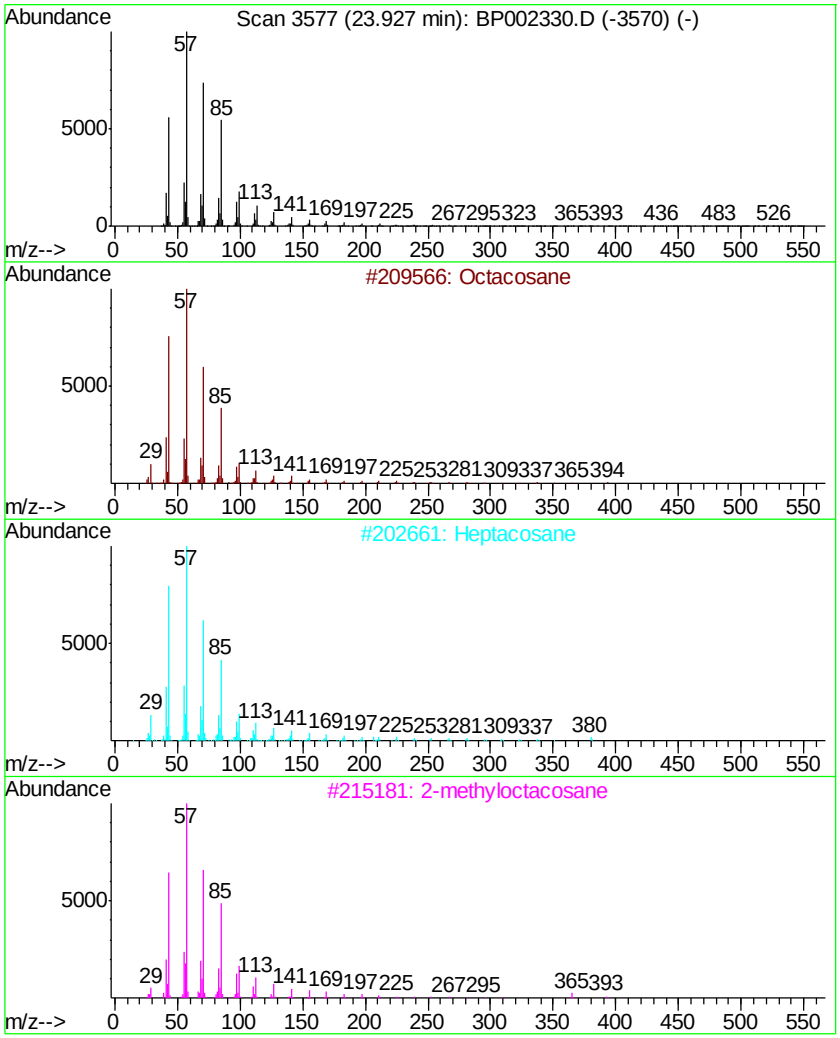
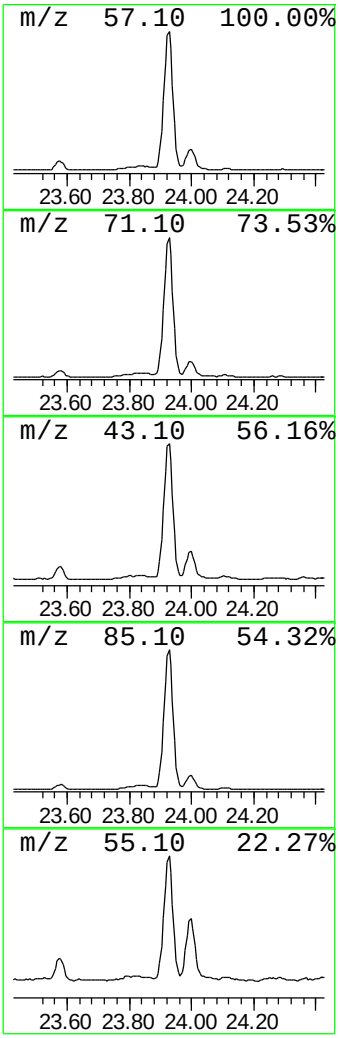
Peak Number 9 Octacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.93	39.51 ng	8042670	Perylene-d12	23.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	98
2	Heptacosane	380	C27H56	000593-49-7	93
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002330.D
Acq On : 29 May 2020 23:43
Operator : CG/JU
Sample : L2745-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM80-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.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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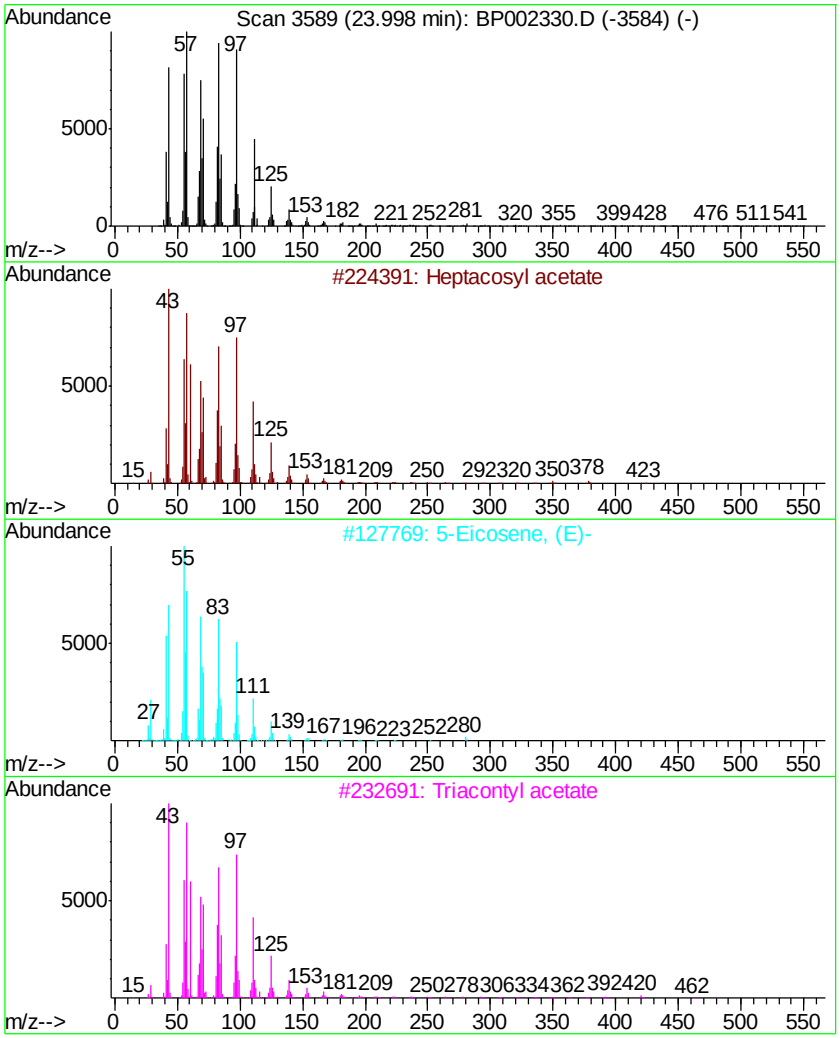
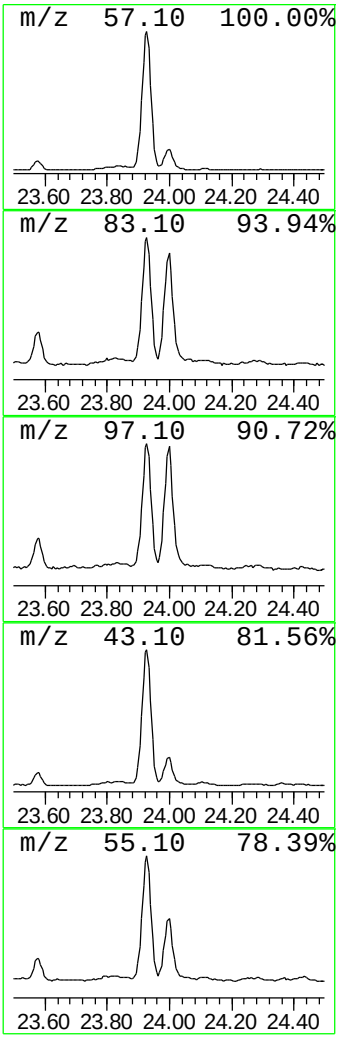
Peak Number 10 Heptacosyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.00	10.70 ng	2178090	Perylene-d12	23.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosyl acetate	438	C29H58O2	1000351-78-2	98
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
3	Triacontyl acetate	480	C32H64O2	041755-58-2	96
4	1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	96
5	1-Heptacosanol	396	C27H56O	002004-39-9	95





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002330.D
Acq On : 29 May 2020 23:43
Operator : CG/JU
Sample : L2745-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM80-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.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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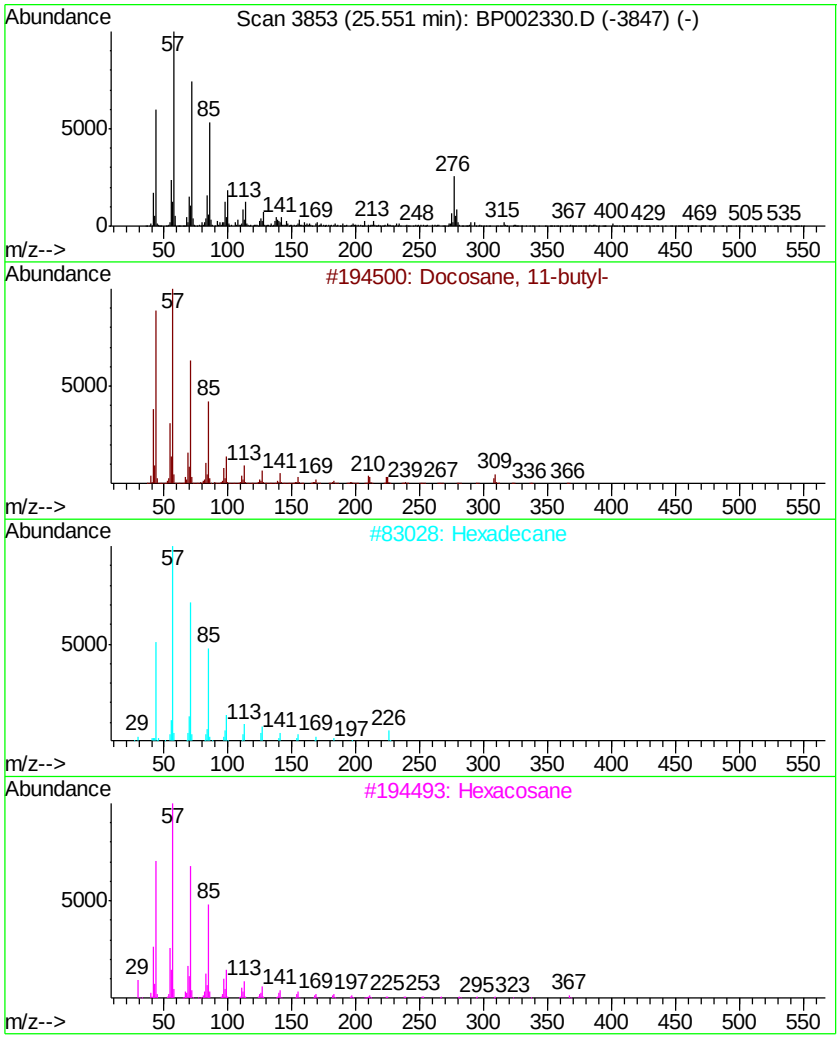
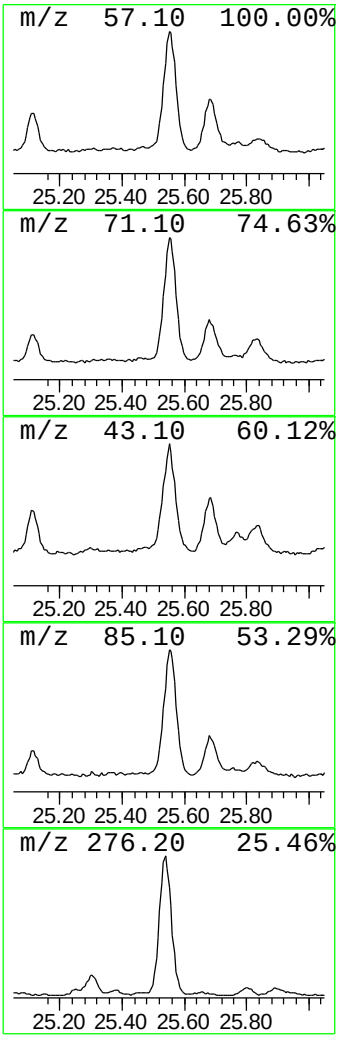
Peak Number 11 Docosane, 11-butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.55	12.34 ng	2512220	Perylene-d12	23.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-	366	C26H54	013475-76-8	90
2	Hexadecane	226	C16H34	000544-76-3	89
3	Hexacosane	366	C26H54	000630-01-3	81
4	Tridecane, 6-propyl-	226	C16H34	055045-10-8	74
5	Tetracosane	338	C24H50	000646-31-1	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002330.D
Acq On : 29 May 2020 23:43
Operator : CG/JU
Sample : L2745-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM80-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.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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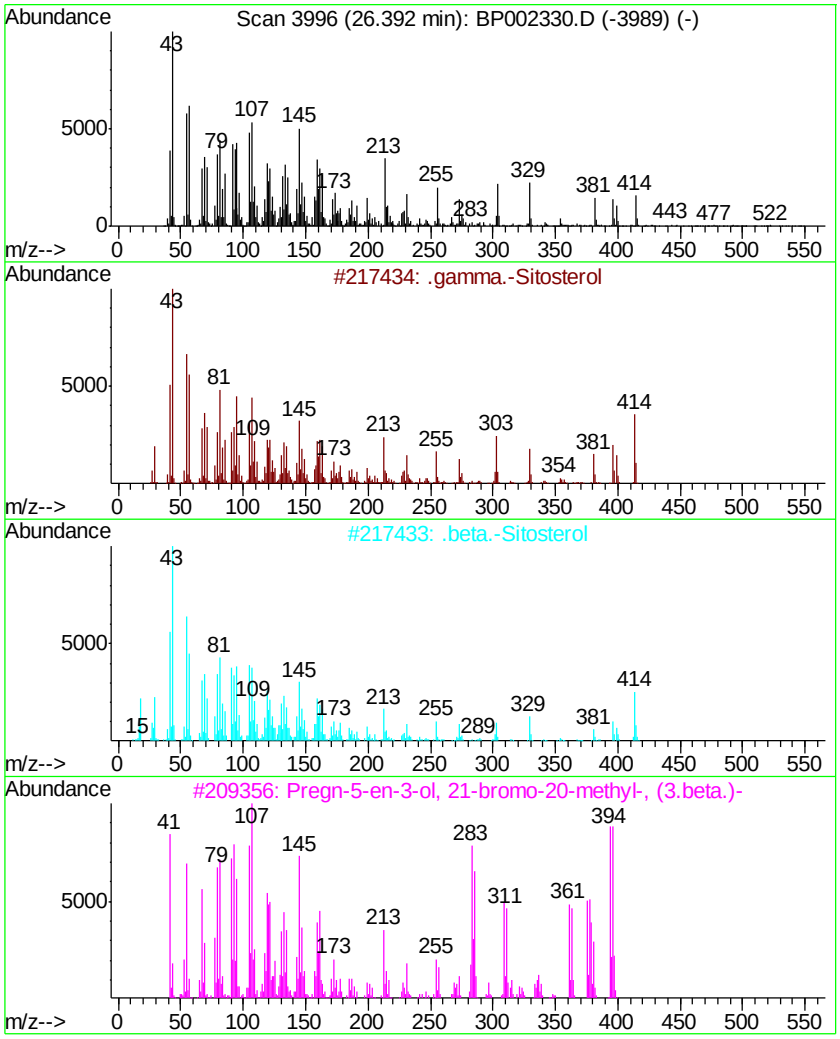
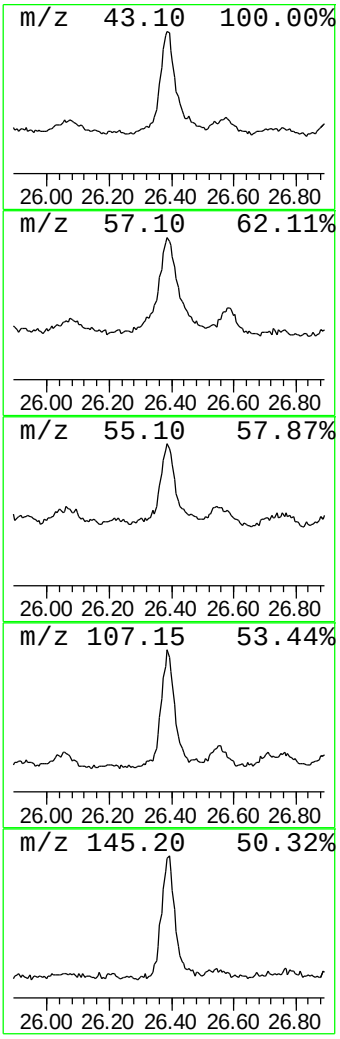
Peak Number 12 .gamma.-Sitosterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.39	13.50 ng	2748720	Perylene-d12	23.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	95
3	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	94
4	Campesterol	400	C28H48O	000474-62-4	47
5	Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP052920\
Data File : BP002330.D
Acq On : 29 May 2020 23:43
Operator : CG/JU
Sample : L2745-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM80-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.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
Butanoic acid, 3-...	4.55	7.9	ng	762602	1	7.60	1927780	20.0
n-Hexadecanoic acid	17.95	6.8	ng	1446480	4	17.01	4224980	20.0
n-Nonadecanol-1	20.86	8.8	ng	2035540	5	21.11	4637770	20.0
5-Octadecene, (E)-	21.74	6.5	ng	1504140	5	21.11	4637770	20.0
17-Octadecenal	22.42	5.5	ng	1119880	6	23.32	4071670	20.0
Cyclotetracosane	22.73	12.7	ng	2586960	6	23.32	4071670	20.0
Octadecanal	23.57	5.3	ng	1085660	6	23.32	4071670	20.0
Octacosane	23.93	39.5	ng	8042670	6	23.32	4071670	20.0
Heptacosyl acetate	24.00	10.7	ng	2178090	6	23.32	4071670	20.0
Docosane, 11-butyl-	25.55	12.3	ng	2512220	6	23.32	4071670	20.0
.gamma.-Sitosterol	26.39	13.5	ng	2748720	6	23.32	4071670	20.0