LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061224\
Data File : BP020604.D
Acq On : 12 Jun 2024 17:29
Operator : MA/JU
Sample : P2812-01 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-05-061024

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: BP020604.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.028	3	7	23	rVB	1047558	1730292	27.33%	3.506%
2	4.923	322	329	336	rBV2	123344	198907	3.14%	0.403%
3	5.370	398	405	425	rBV	1997025	3052018	48.20%	6.185%
4	6.928	662	670	688	rBV	1969634	3136357	49.53%	6.356%
5	7.752	802	810	817	rBV	848688	1444634	22.82%	2.927%
6	8.899	997	1005	1013	rBV	1107373	2020568	31.91%	4.095%
7	9.452	1094	1099	1112	rVB	43615	79306	1.25%	0.161%
8	10.510	1268	1279	1286	rBV	1176646	1998202	31.56%	4.049%
9	11.257	1401	1406	1417	rVB2	37417	79168	1.25%	0.160%
10	12.975	1691	1698	1715	rBV	3266038	4712378	74.43%	9.549%
11	14.269	1913	1918	1925	rBV	61130	93343	1.47%	0.189%
12	14.375	1926	1936	1942	rBV	1717729	2603401	41.12%	5.276%
13	14.434	1942	1946	1953	rVB3	52583	100236	1.58%	0.203%
14	14.587	1967	1972	1981	rVB5	36865	102740	1.62%	0.208%
15	14.787	2001	2006	2013	rVB3	44129	77234	1.22%	0.157%
16	15.240	2080	2083	2091	rVB	68066	107209	1.69%	0.217%
17	15.440	2113	2117	2121	rBV2	57812	81930	1.29%	0.166%
18	15.651	2149	2153	2159	rVB2	42781	68747	1.09%	0.139%
19	15.887	2187	2193	2203	rBV	2269721	3481468	54.99%	7.055%
20	16.134	2231	2235	2238	rBV2	109330	170876	2.70%	0.346%
21	16.945	2369	2373	2377	rBV	88698	119970	1.89%	0.243%
22	16.998	2378	2382	2390	rVB2	96566	158609	2.51%	0.321%
23	17.175	2406	2412	2417	rBV	1924300	2922922	46.16%	5.923%
24	17.216	2417	2419	2426	rVB	346373	470595	7.43%	0.954%
25	17.316	2433	2436	2442	rVB	72841	121226	1.91%	0.246%
26	17.598	2481	2484	2488	rBV3	35504	65011	1.03%	0.132%
27	17.710	2499	2503	2509	rBV2	103678	133454	2.11%	0.270%
28	17.887	2529	2533	2537	rBV	108826	135490	2.14%	0.275%
29	18.087	2563	2567	2569	rBV	78661	113978	1.80%	0.231%
30	18.122	2569	2573	2584	rVB2	967949	1376092	21.73%	2.789%
31	18.281	2596	2600	2605	rBV2	100280	189166	2.99%	0.383%
32	18.434	2623	2626	2631	rBV2	107988	138276	2.18%	0.280%
33	18.916	2705	2708	2712	rBV2	60028	67844	1.07%	0.137%
34	19.034	2724	2728	2732	rBV	127923	217468	3.43%	0.441%
35	19.086	2732	2737	2740	rVV3	469391	798364	12.61%	1.618%
36	19.122	2740	2743	2750	rVB4	297237	447897	7.07%	0.908%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061224\
Data File : BP020604.D
Acq On : 12 Jun 2024 17:29
Operator : MA/JU
Sample : P2812-01 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-05-061024

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

37	19.257	2763	2766	2770	rVB3	87596	107108	1.69%	0.217%
38	19.316	2771	2776	2781	rBV	706270	972277	15.36%	1.970%
39	19.469	2797	2802	2810	rBV2	523963	840826	13.28%	1.704%
40	19.698	2833	2841	2850	rBV	720039	1228092	19.40%	2.489%
41	19.922	2873	2879	2889	rVB	4452941	6331627	100.00%	12.831%
42	20.263	2934	2937	2940	rBV	128619	138010	2.18%	0.280%
43	21.328	3114	3118	3129	rVB3	340315	611688	9.66%	1.240%
44	21.639	3165	3171	3176	rBV3	1831435	3158835	49.89%	6.401%
45	24.998	3735	3742	3752	rVB2	1158665	3144209	49.66%	6.371%

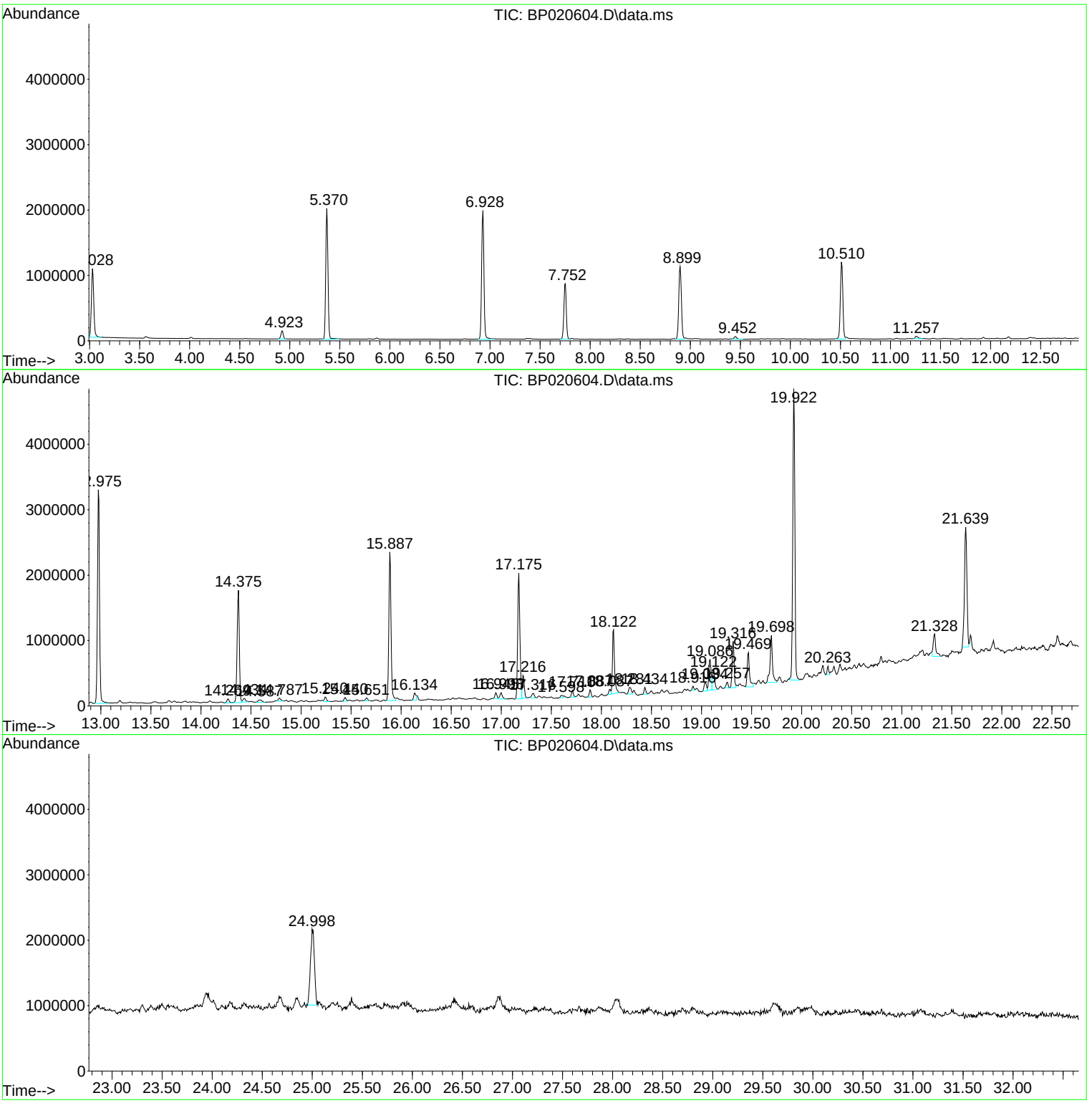
Sum of corrected areas: 49348048

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061224\
Data File : BP020604.D
Acq On : 12 Jun 2024 17:29
Operator : MA/JU
Sample : P2812-01 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-05-061024

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061224\
Data File : BP020604.D
Acq On : 12 Jun 2024 17:29
Operator : MA/JU
Sample : P2812-01 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-05-061024

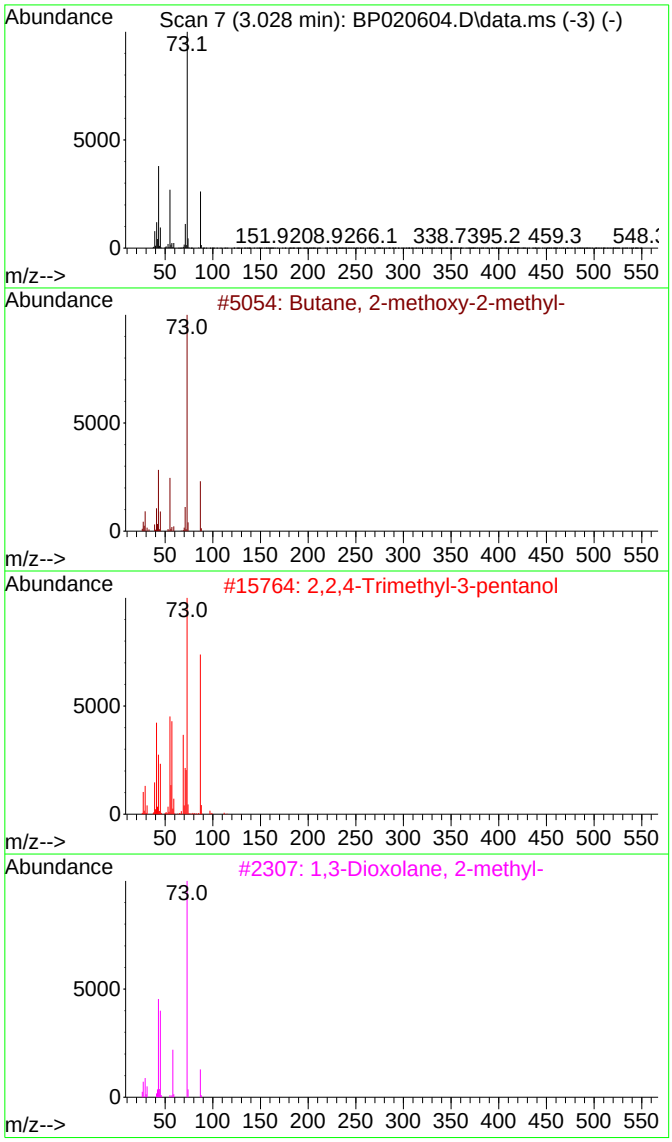
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

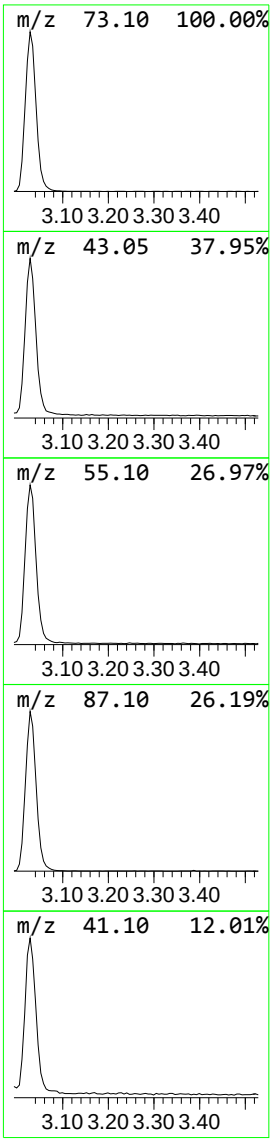
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.028	23.95 ng	1730290	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	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061224\
Data File : BP020604.D
Acq On : 12 Jun 2024 17:29
Operator : MA/JU
Sample : P2812-01 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-05-061024

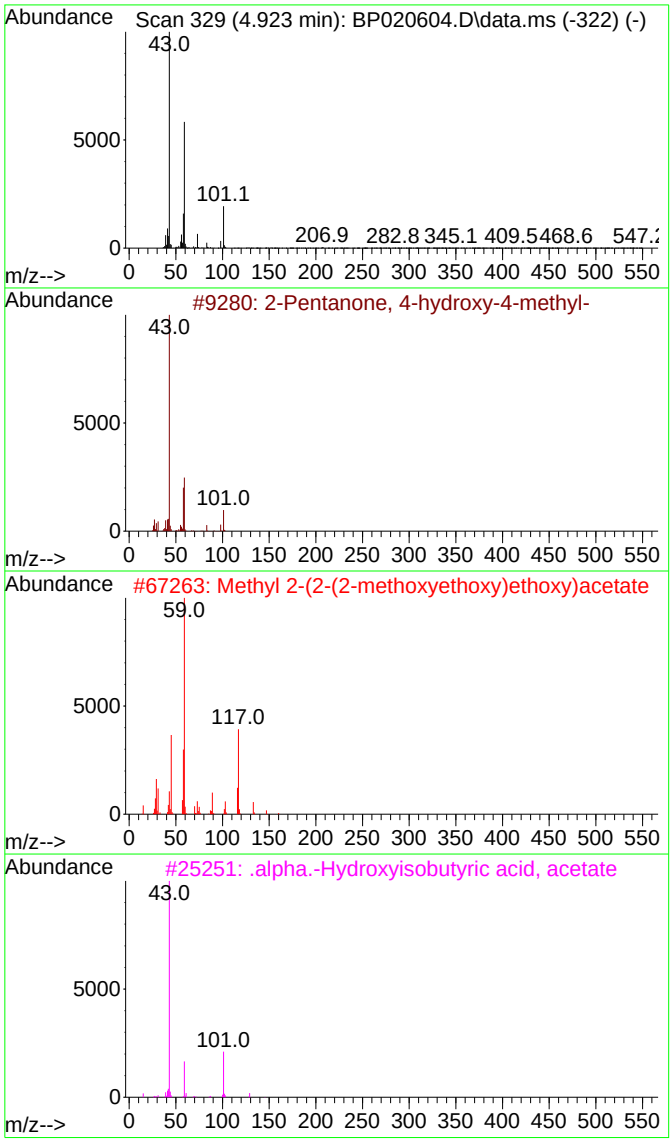
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

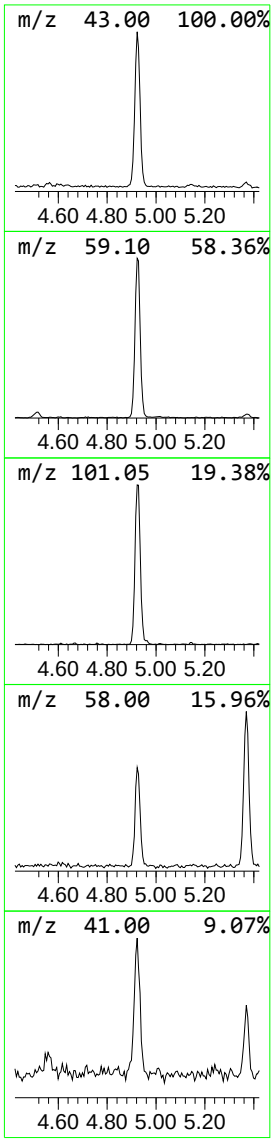
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.923	2.75 ng	198907	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	64
2	Methyl 2-(2-(2-methoxyethoxy)eth...	192	C8H16O5	1000366-88-2	25
3	.alpha.-Hydroxyisobutyric acid, ...	146	C6H10O4	1000374-31-3	17
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061224\
Data File : BP020604.D
Acq On : 12 Jun 2024 17:29
Operator : MA/JU
Sample : P2812-01 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-05-061024

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

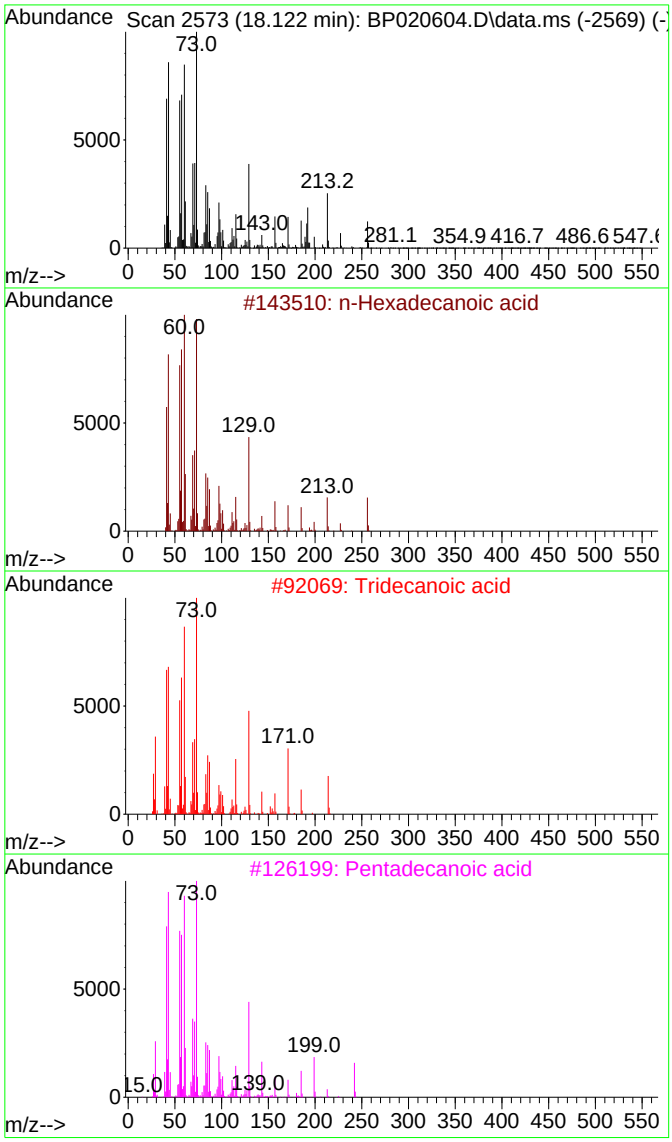
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

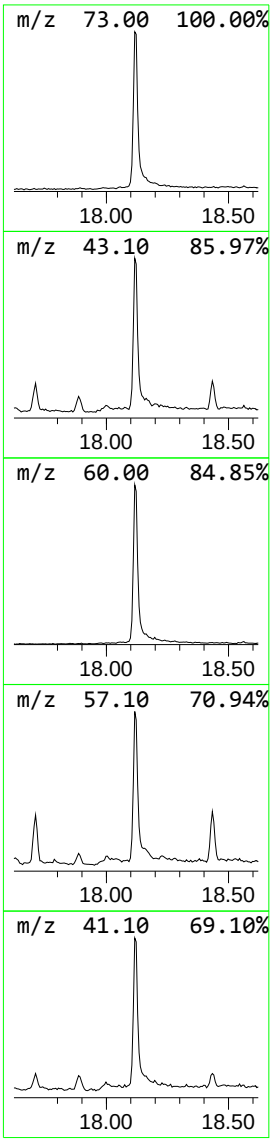
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.122	9.42 ng	1376090	Phenanthrene-d10	17.175

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061224\
Data File : BP020604.D
Acq On : 12 Jun 2024 17:29
Operator : MA/JU
Sample : P2812-01 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-05-061024

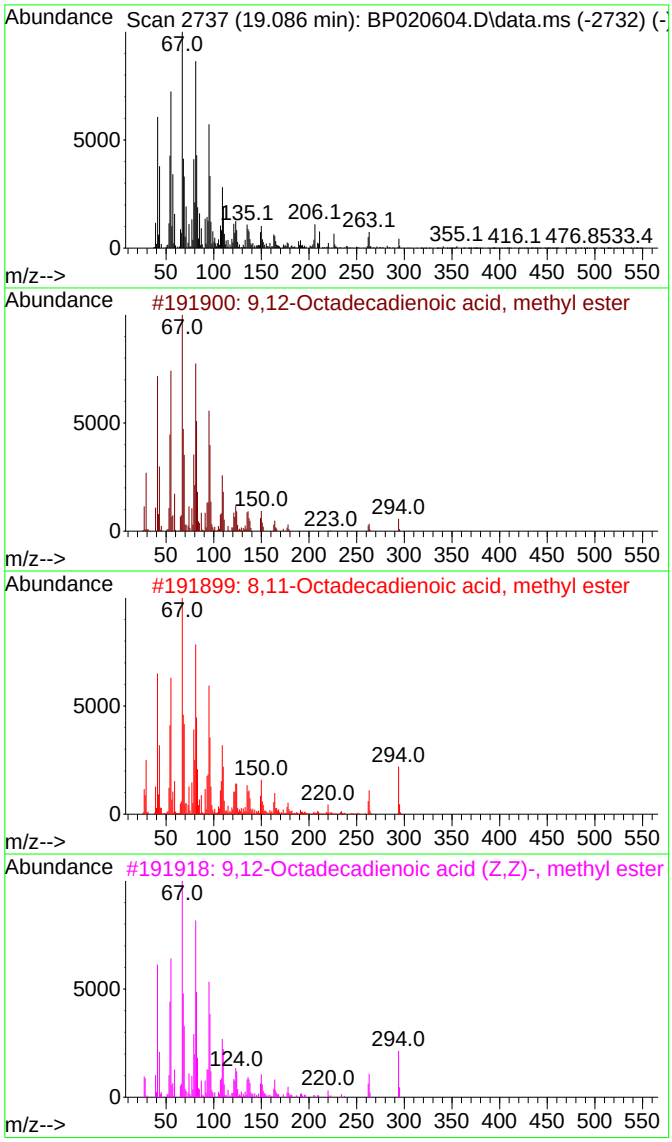
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

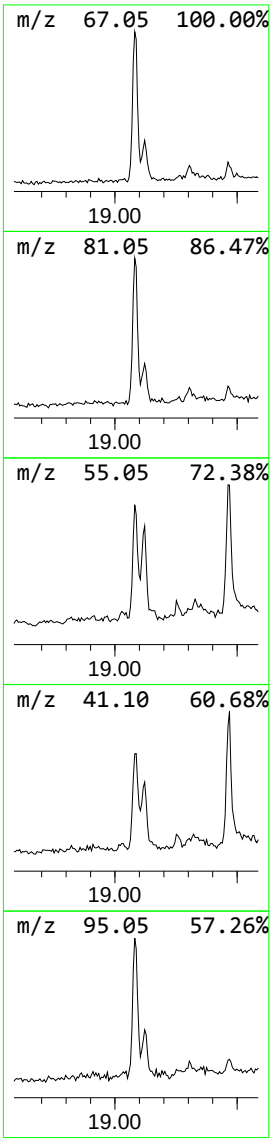
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.086	5.46 ng	798364	Phenanthrene-d10	17.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	98
5	9,17-Octadecadienal, (Z)-	264	C18H32O	056554-35-9	98





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061224\
Data File : BP020604.D
Acq On : 12 Jun 2024 17:29
Operator : MA/JU
Sample : P2812-01 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-05-061024

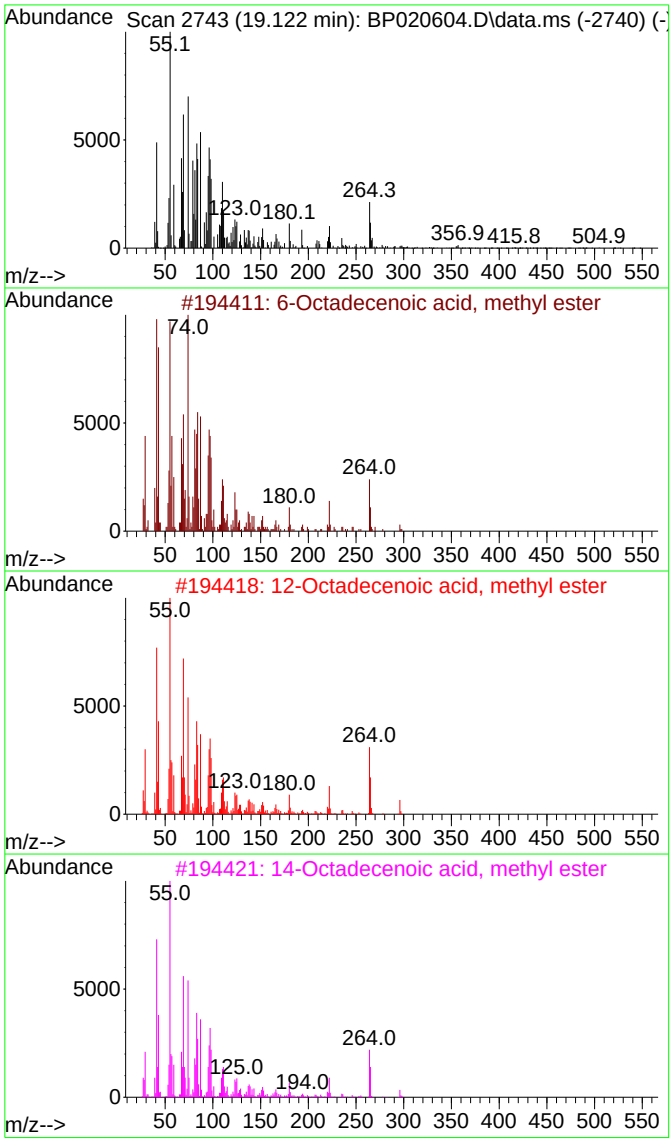
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

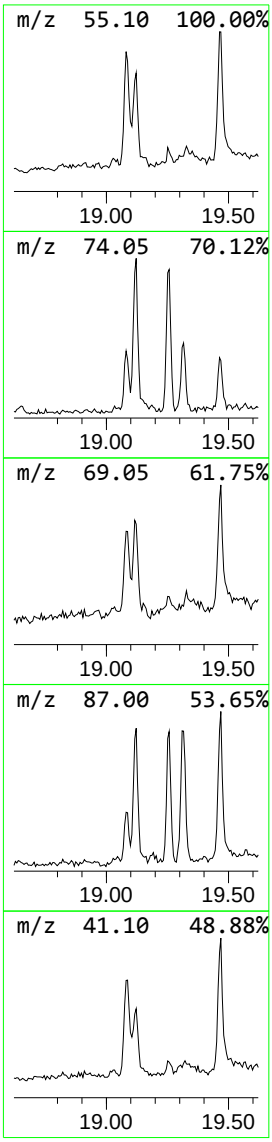
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 6-Octadecenoic acid, methyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.122	3.06 ng	447897	Phenanthrene-d10	17.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	94
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	94
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	93
4	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	93
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	92





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061224\
Data File : BP020604.D
Acq On : 12 Jun 2024 17:29
Operator : MA/JU
Sample : P2812-01 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-05-061024

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

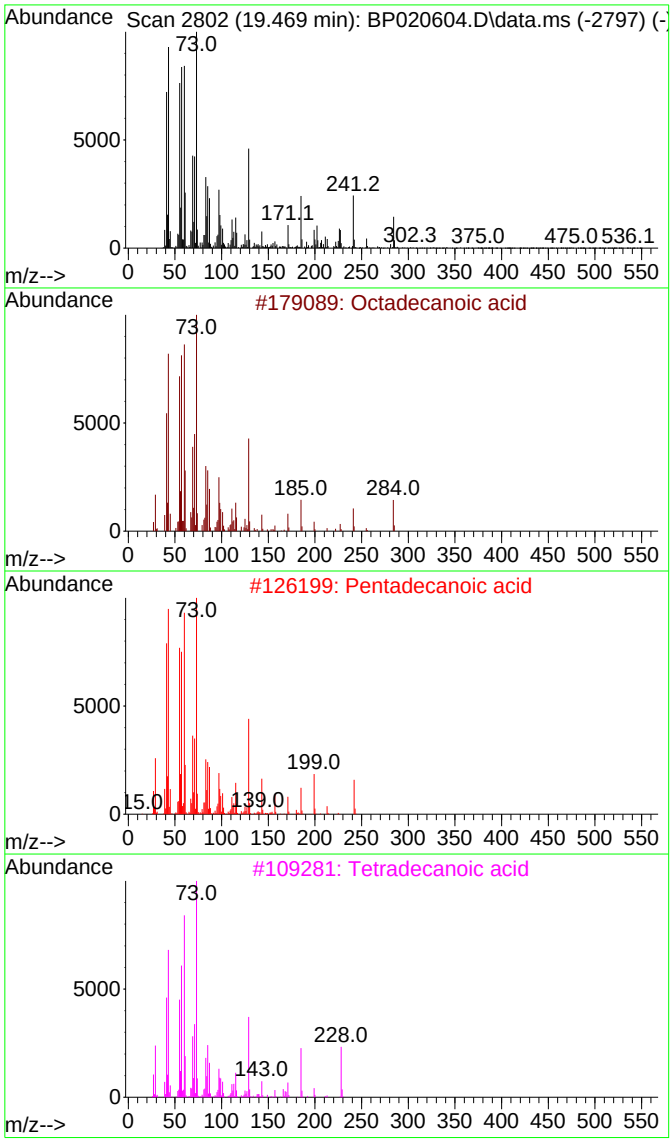
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

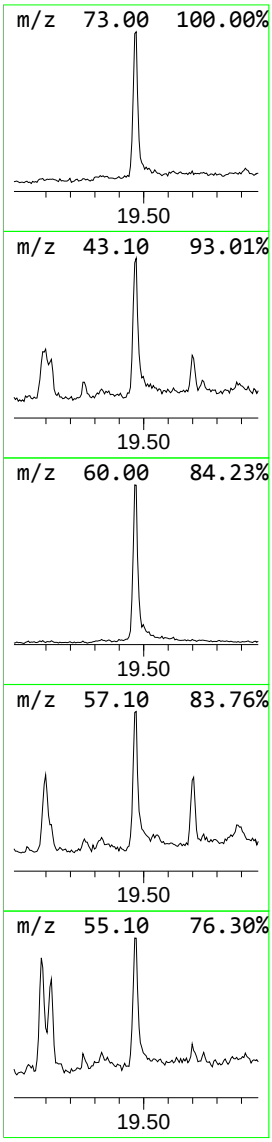
****

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.469	5.32 ng	840826	Chrysene-d12	21.639

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	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061224\
Data File : BP020604.D
Acq On : 12 Jun 2024 17:29
Operator : MA/JU
Sample : P2812-01 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-05-061024

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

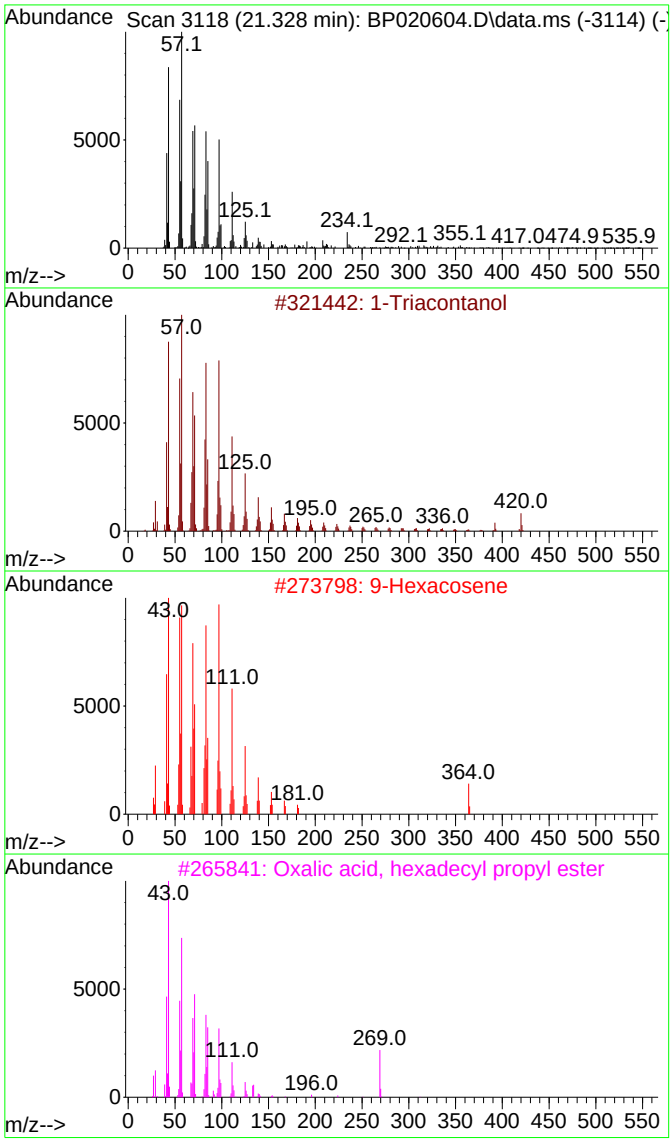
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

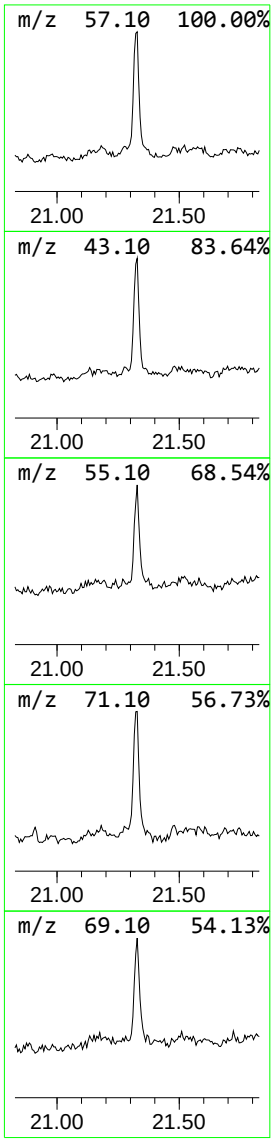
****

Peak Number 7 1-Triacontanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.328	3.87 ng	611688	Chrysene-d12	21.639

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Triacontanol	438	C30H62O	000593-50-0	93
2	9-Hexacosene	364	C26H52	071502-22-2	93
3	Oxalic acid, hexadecyl propyl ester	356	C21H40O4	1000309-26-9	91
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061224\
Data File : BP020604.D
Acq On : 12 Jun 2024 17:29
Operator : MA/JU
Sample : P2812-01 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-05-061024

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...	3.028	23.9	ng	1730290	1	7.752	1444630	20.0
2-Pentanone, 4-...	4.923	2.8	ng	198907	1	7.752	1444630	20.0
n-Hexadecanoic ...	18.122	9.4	ng	1376090	4	17.175	2922920	20.0
9,12-Octadecadi...	19.086	5.5	ng	798364	4	17.175	2922920	20.0
6-Octadecenoic ...	19.122	3.1	ng	447897	4	17.175	2922920	20.0
Octadecanoic acid	19.469	5.3	ng	840826	5	21.639	3158840	20.0
1-Triacontanol	21.328	3.9	ng	611688	5	21.639	3158840	20.0