LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111119\
Data File : BP001024.D
Acq On : 11 Nov 2019 19:11
Operator : JU
Sample : K5760-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-50

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-BP110619.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	2.317	33	39	49	rVB	647461	973307	15.48%	1.714%
2	5.734	615	620	636	rVB	475211	712633	11.33%	1.255%
3	6.305	711	717	722	rBV	3247138	4111011	65.37%	7.239%
4	7.816	967	974	982	rBV	3510120	4658027	74.07%	8.202%
5	8.010	1001	1007	1012	rBV	3796259	4701091	74.76%	8.278%
6	8.375	1063	1069	1074	rVB	1227186	1419308	22.57%	2.499%
7	8.616	1104	1110	1114	rBV	3200661	3844174	61.13%	6.769%
8	9.246	1210	1217	1221	rBV	2339586	2833869	45.06%	4.990%
9	10.398	1408	1413	1418	rBV	1576828	1804309	28.69%	3.177%
10	12.181	1709	1716	1720	rBV	4981052	5985776	95.19%	10.540%
11	12.839	1824	1828	1833	rVB	296240	338586	5.38%	0.596%
12	13.263	1894	1900	1905	rBV	1891458	2261827	35.97%	3.983%
13	14.551	2113	2119	2134	rBV	3487749	4337014	68.97%	7.637%
14	14.886	2173	2176	2181	rVB	62420	76273	1.21%	0.134%
15	15.622	2297	2301	2302	rBV	93453	108228	1.72%	0.191%
16	15.657	2302	2307	2310	rVV	1936850	2292572	36.46%	4.037%
17	15.686	2310	2312	2318	rVB	165986	169695	2.70%	0.299%
18	16.539	2453	2457	2460	rBV	337101	401921	6.39%	0.708%
19	17.398	2599	2603	2607	rVB	352121	389498	6.19%	0.686%
20	17.627	2639	2642	2646	rBV	72630	90320	1.44%	0.159%
21	17.698	2650	2654	2659	rVB	310280	378845	6.02%	0.667%
22	17.933	2689	2694	2698	rVB	5662152	6288426	100.00%	11.073%
23	19.157	2899	2902	2916	rVB3	533058	771624	12.27%	1.359%
24	19.292	2919	2925	2929	rVV	2139615	2550345	40.56%	4.491%
25	19.322	2929	2930	2935	rVB2	208667	204647	3.25%	0.360%
26	19.586	2972	2975	2980	rBV3	77648	87778	1.40%	0.155%
27	19.974	3038	3041	3046	rVB2	149427	156386	2.49%	0.275%
28	20.351	3103	3105	3114	rVB	358630	565924	9.00%	0.997%
29	20.439	3116	3120	3124	rVB	500581	575886	9.16%	1.014%
30	20.580	3141	3144	3147	rBV	155336	190227	3.03%	0.335%
31	20.757	3171	3174	3186	rVB4	161598	308003	4.90%	0.542%
32	20.927	3201	3203	3207	rVB2	73934	81312	1.29%	0.143%
33	20.998	3212	3215	3220	rVB	178384	235815	3.75%	0.415%
34	21.080	3223	3229	3242	rVB	1651142	2546193	40.49%	4.484%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111119\
Data File : BP001024.D
Acq On : 11 Nov 2019 19:11
Operator : JU
Sample : K5760-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-50

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-BP110619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.204	3247	3250	3256	rVB	116176	172350	2.74%	0.303%
36	21.710	3333	3336	3340	rBV2	132660	165773	2.64%	0.292%

Sum of corrected areas: 56788973

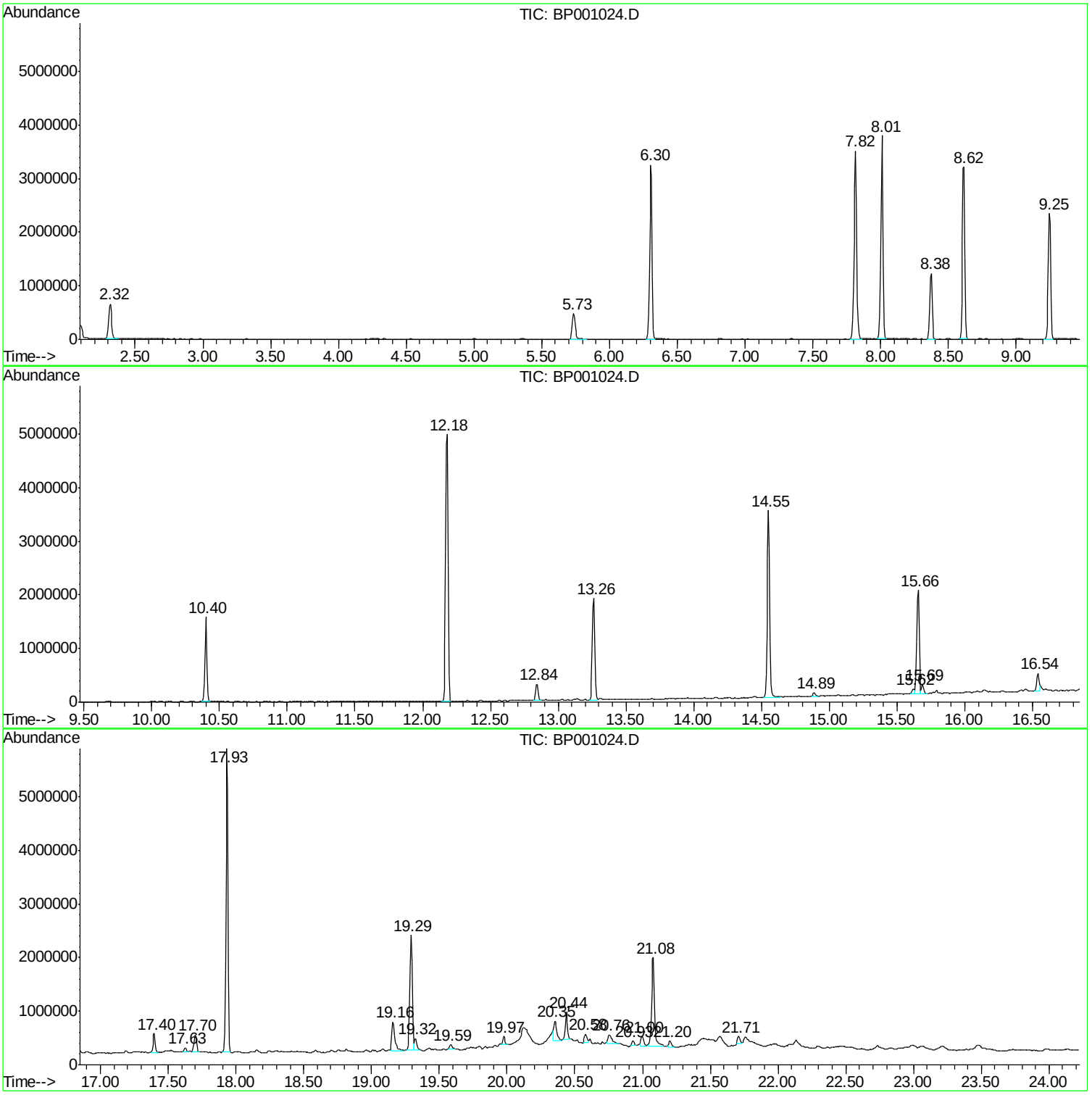
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111119\
Data File : BP001024.D
Acq On : 11 Nov 2019 19:11
Operator : JU
Sample : K5760-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.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\BP111119\
Data File : BP001024.D
Acq On : 11 Nov 2019 19:11
Operator : JU
Sample : K5760-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

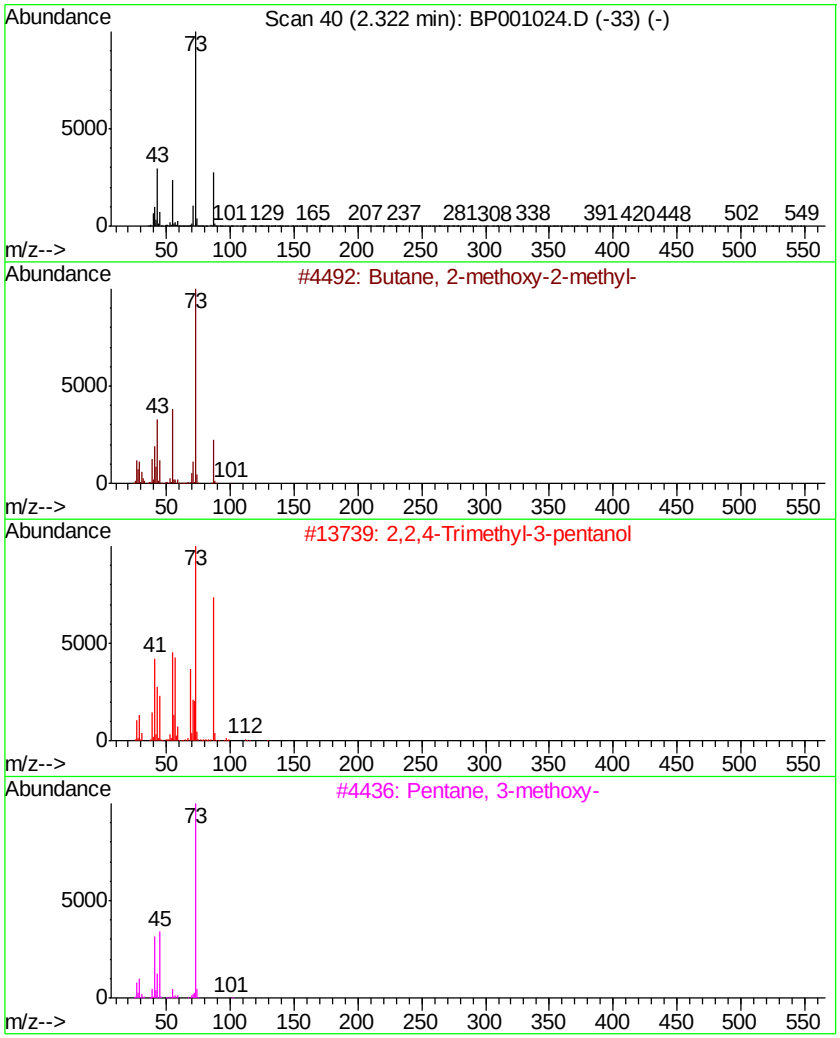
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

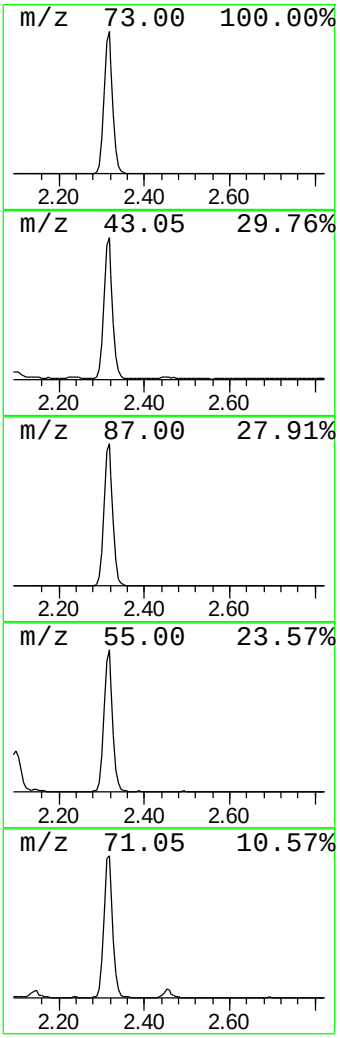
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	13.72 ng	973307	1,4-Dichlorobenzene-d4	8.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111119\
Data File : BP001024.D
Acq On : 11 Nov 2019 19:11
Operator : JU
Sample : K5760-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

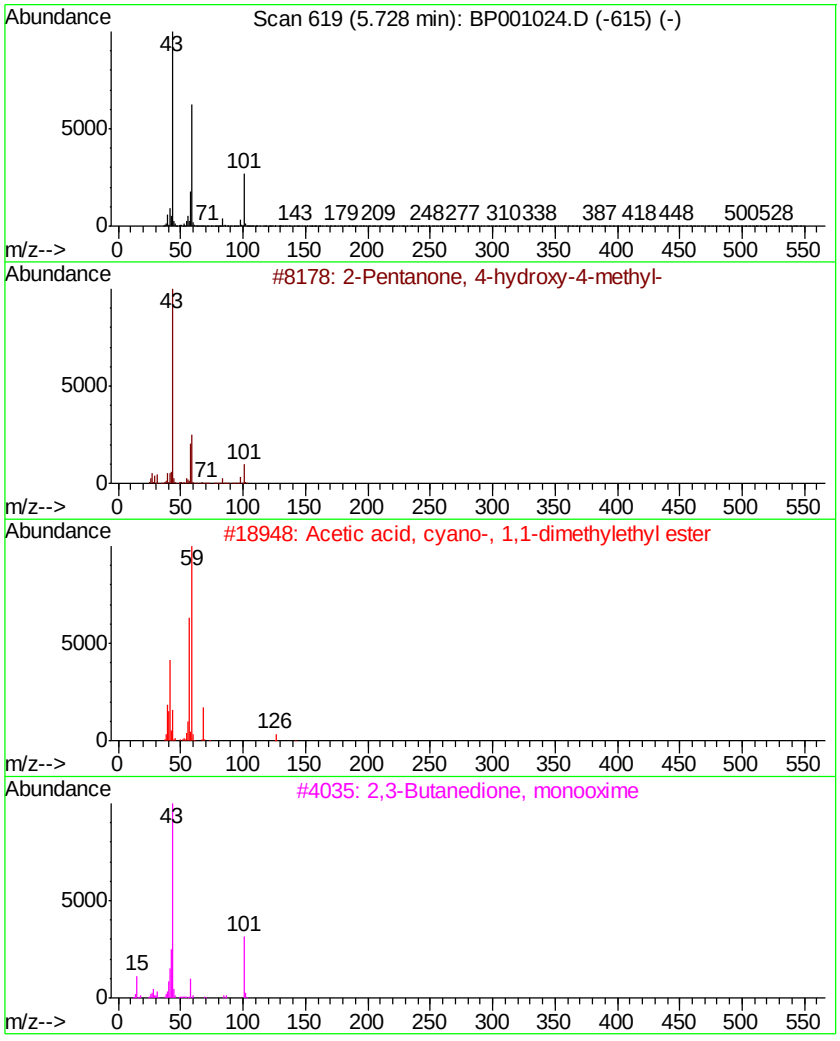
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

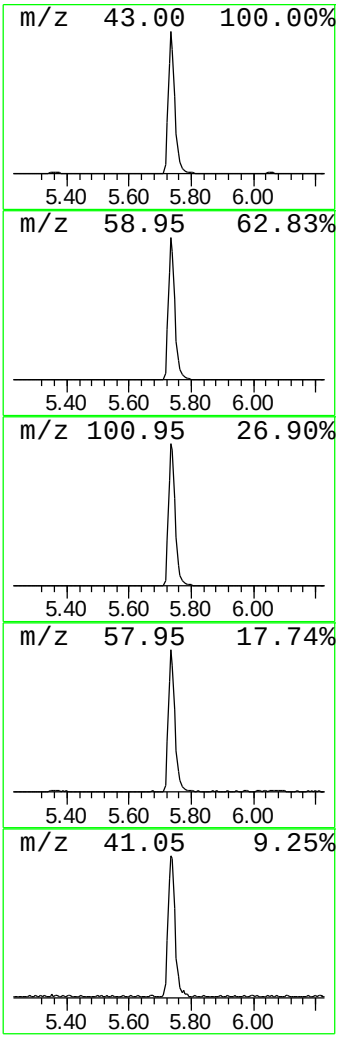
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.73	10.04 ng	712633	1,4-Dichlorobenzene-d4	8.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	Acetone	58	C3H6O	000067-64-1	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111119\
Data File : BP001024.D
Acq On : 11 Nov 2019 19:11
Operator : JU
Sample : K5760-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

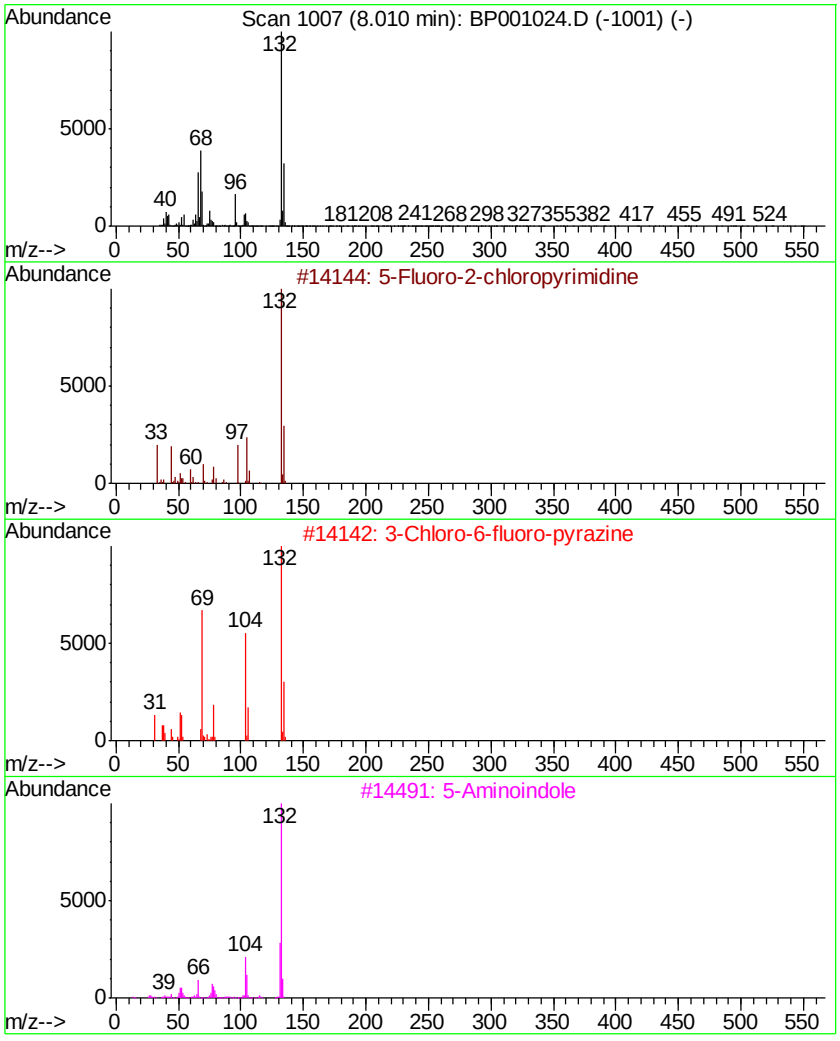
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

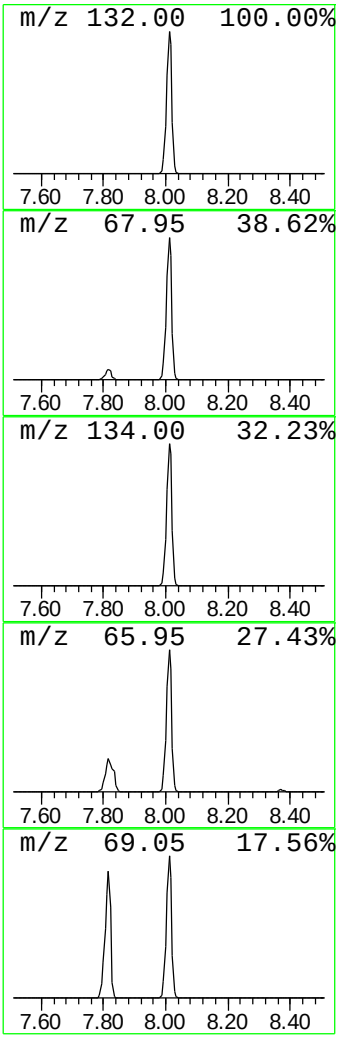
****

Peak Number 3 unknown8.01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.01	66.24 ng	4701090	1,4-Dichlorobenzene-d4	8.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10
5	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111119\
Data File : BP001024.D
Acq On : 11 Nov 2019 19:11
Operator : JU
Sample : K5760-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

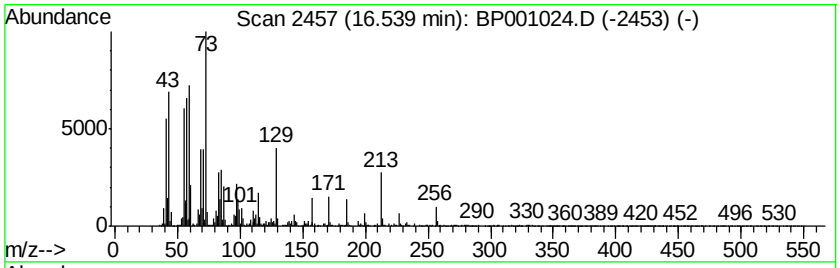
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

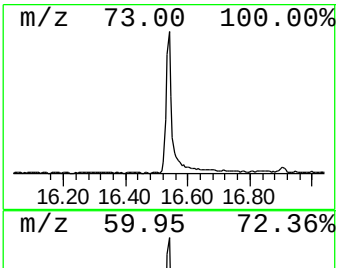
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.54	3.51 ng	401921	Phenanthrene-d10	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Octadecanoic acid	284	C18H36O2	000057-11-4	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111119\
Data File : BP001024.D
Acq On : 11 Nov 2019 19:11
Operator : JU
Sample : K5760-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

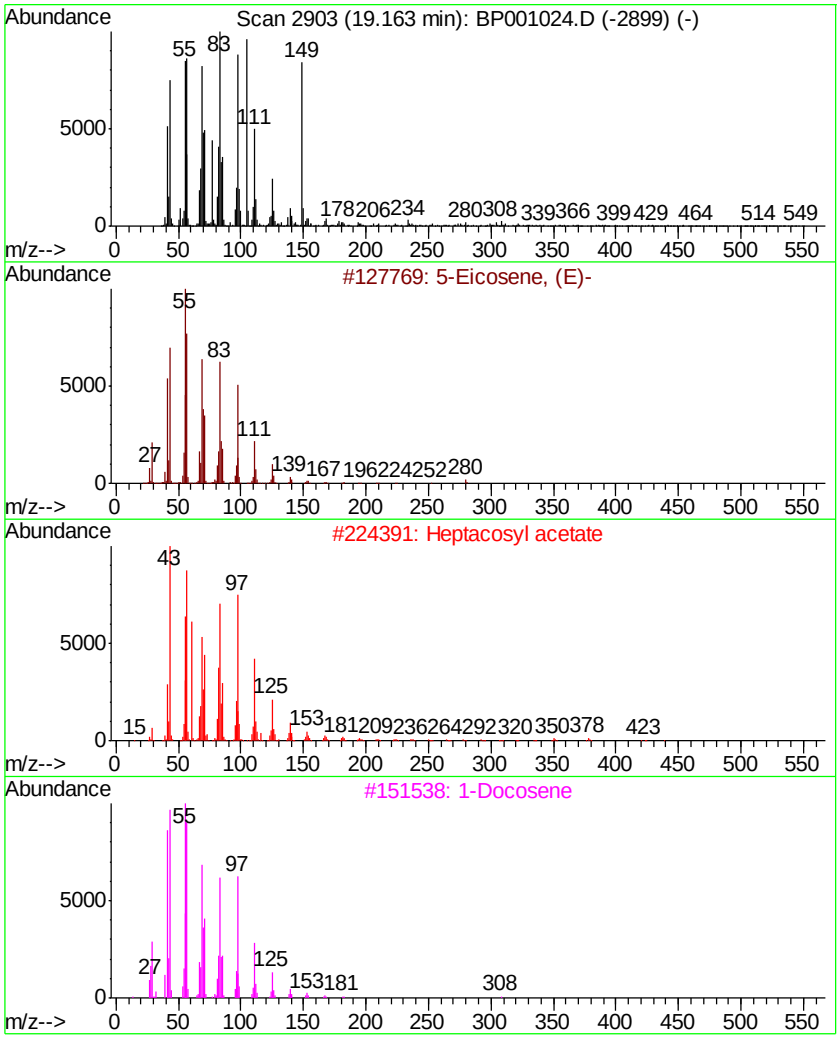
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

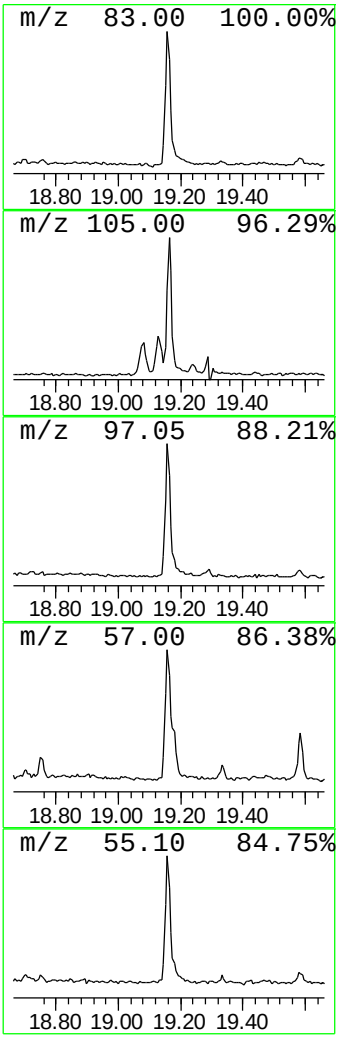
****

Peak Number 6 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.16	6.05 ng	771624	Chrysene-d12	19.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	Heptacosyl acetate	438	C29H58O2	1000351-78-2	96
3	1-Docosene	308	C22H44	001599-67-3	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Behenic alcohol	326	C22H46O	000661-19-8	93





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111119\
Data File : BP001024.D
Acq On : 11 Nov 2019 19:11
Operator : JU
Sample : K5760-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

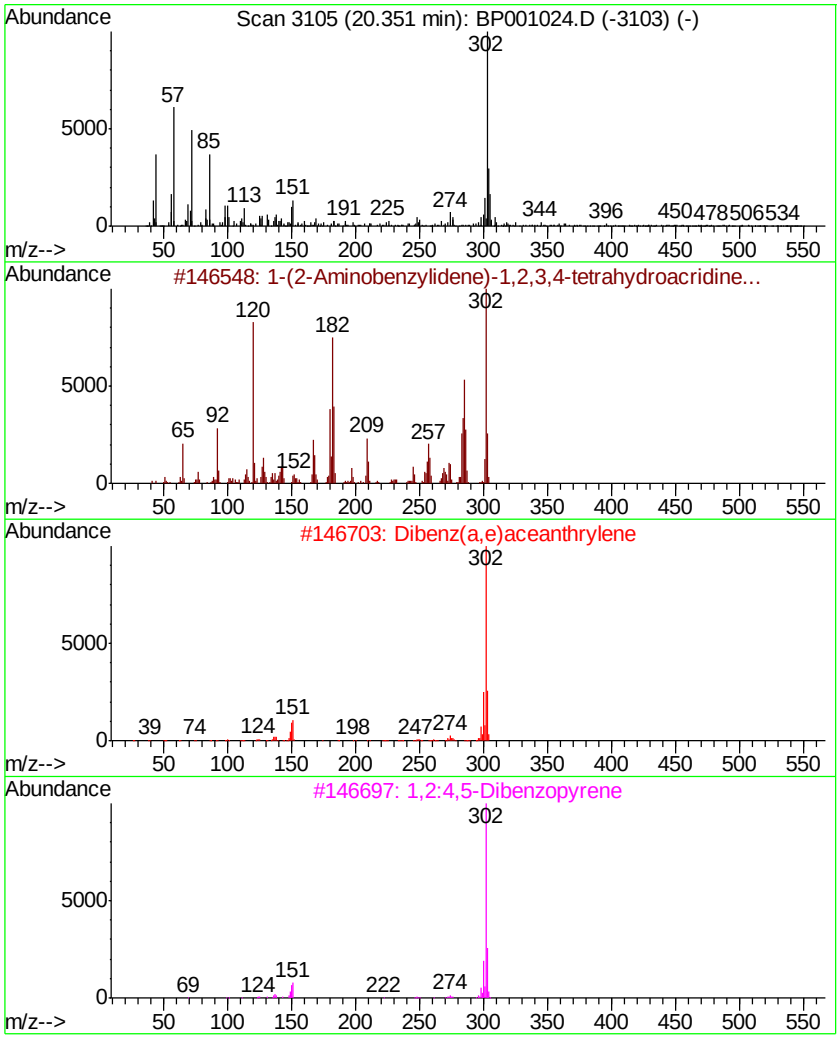
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

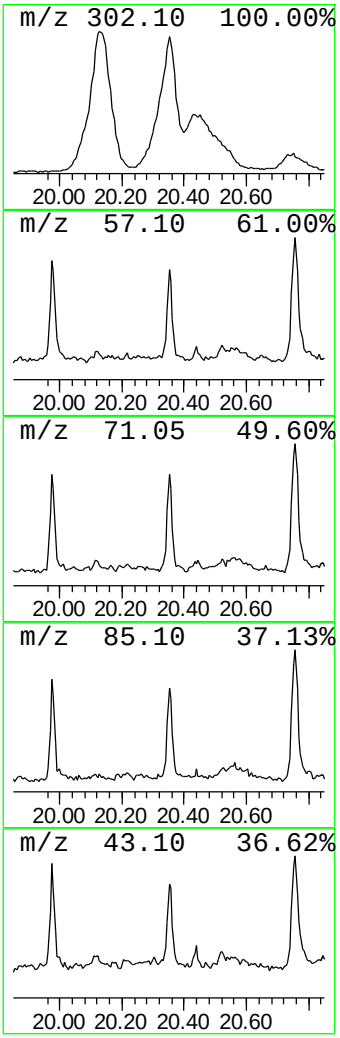
****

Peak Number 7 1-(2-Aminobenzylidene)-1,2,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.35	4.45 ng	565924	Perylene-d12	21.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Aminobenzylidene)-1,2,3,4-t...	302	C20H18N2O	1000110-40-2	95
2	Dibenz(a,e)aceanthrylene	302	C24H14	005385-75-1	72
3	1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	64
4	Dibenzo(a,i)pyrene	302	C24H14	000189-55-9	64
5	3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111119\
Data File : BP001024.D
Acq On : 11 Nov 2019 19:11
Operator : JU
Sample : K5760-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

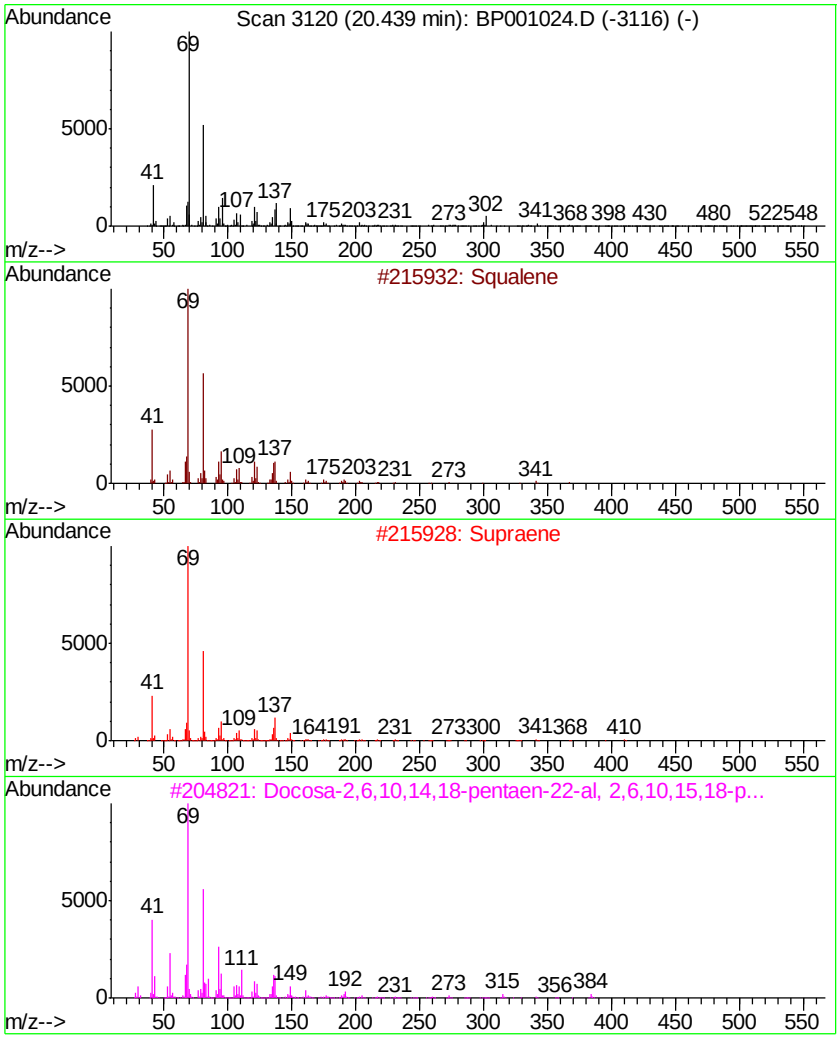
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

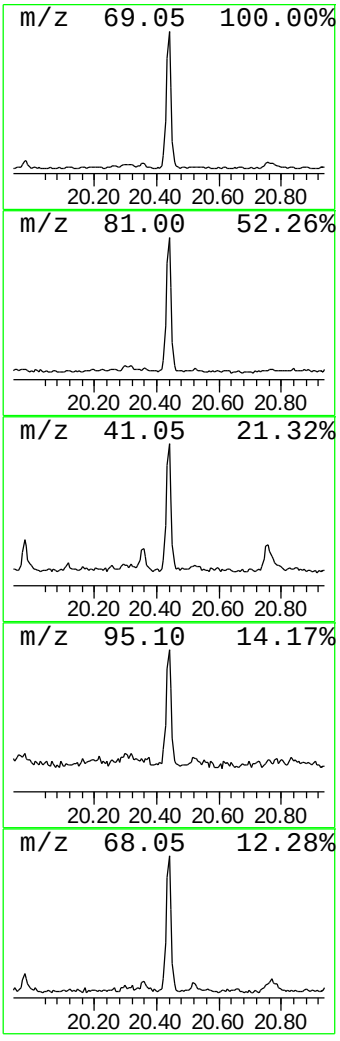
****

Peak Number 8 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.44	4.52 ng	575886	Perylene-d12	21.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	87
2	Supraene	410	C30H50	007683-64-9	87
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
4	Farnesol isomer a	222	C15H26O	1000108-92-4	64
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111119\
Data File : BP001024.D
Acq On : 11 Nov 2019 19:11
Operator : JU
Sample : K5760-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

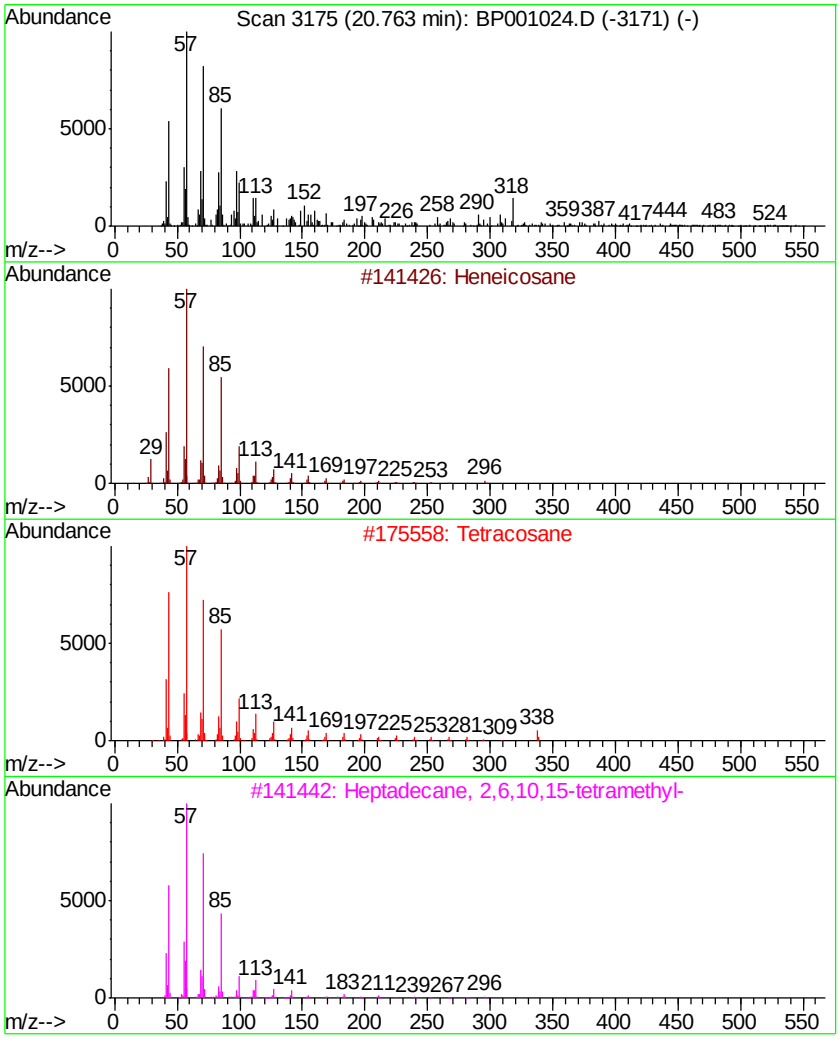
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

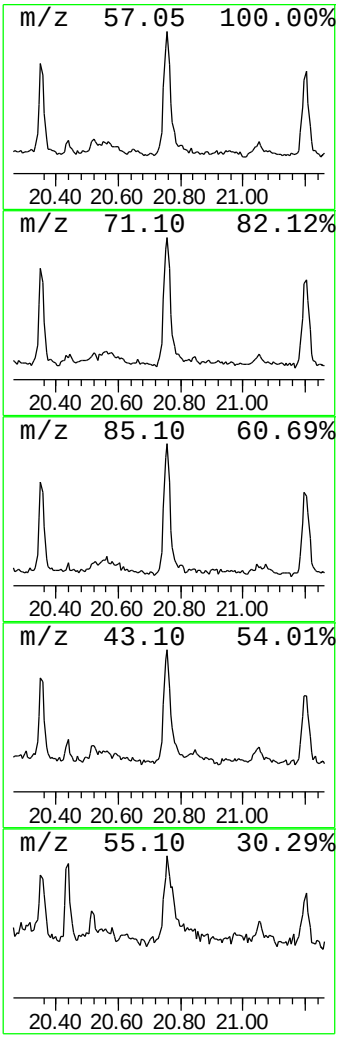
****

Peak Number 9 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.76	2.42 ng	308003	Perylene-d12	21.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Tetracosane	338	C24H50	000646-31-1	93
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
4	Heptacosane	380	C27H56	000593-49-7	90
5	Tricosane, 2-methyl-	338	C24H50	001928-30-9	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP111119\
Data File : BP001024.D
Acq On : 11 Nov 2019 19:11
Operator : JU
Sample : K5760-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : RBR-50

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.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
Butane, 2-methoxy...	2.32	13.7	ng	973307	1	8.38	1419310	20.0
2-Pentanone, 4-hy...	5.73	10.0	ng	712633	1	8.38	1419310	20.0
unknown8.01	8.01	66.2	ng	4701090	1	8.38	1419310	20.0
n-Hexadecanoic acid	16.54	3.5	ng	401921	4	15.66	2292570	20.0
5-Eicosene, (E)-	19.16	6.0	ng	771624	5	19.29	2550350	20.0
1-(2-Aminobenzyli...	20.35	4.5	ng	565924	6	21.08	2546190	20.0
Squalene	20.44	4.5	ng	575886	6	21.08	2546190	20.0
Tetracosane	20.76	2.4	ng	308003	6	21.08	2546190	20.0