LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
Data File : BP001052.D
Acq On : 15 Nov 2019 21:26
Operator : JU
Sample : K5832-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 6-(6-8)

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	2.346	37	44	54	rVB	412829	634019	8.60%	1.123%
2	5.740	616	621	637	rVB	425303	661827	8.98%	1.172%
3	6.310	710	718	722	rBV	3050231	3869196	52.49%	6.851%
4	7.816	966	974	987	rVB	3065431	4196571	56.93%	7.431%
5	8.010	1000	1007	1011	rBV	3410606	4423935	60.02%	7.834%
6	8.363	1062	1067	1073	rBV	1055773	1259272	17.08%	2.230%
7	8.604	1102	1108	1113	rBV	3013311	3696942	50.15%	6.546%
8	9.240	1209	1216	1220	rBV	2127465	2654551	36.01%	4.700%
9	10.393	1406	1412	1417	rBV	1354602	1604424	21.77%	2.841%
10	12.169	1705	1714	1719	rBV	4976500	6095254	82.69%	10.793%
11	12.834	1821	1827	1835	rBV	658801	756521	10.26%	1.340%
12	13.251	1891	1898	1904	rBV	1652361	2045850	27.76%	3.623%
13	14.545	2110	2118	2131	rBV	3562247	4456827	60.46%	7.892%
14	15.645	2295	2305	2309	rBV	2015564	2284412	30.99%	4.045%
15	15.681	2309	2311	2316	rVB	251418	236021	3.20%	0.418%
16	15.786	2326	2329	2334	rVB	79931	91423	1.24%	0.162%
17	16.439	2436	2440	2446	rVB	64925	79846	1.08%	0.141%
18	16.528	2447	2455	2457	rBV2	234087	290833	3.95%	0.515%
19	16.833	2503	2507	2513	rVB2	51718	83152	1.13%	0.147%
20	17.386	2596	2601	2605	rBV	435218	451893	6.13%	0.800%
21	17.610	2637	2639	2644	rBV2	67346	78609	1.07%	0.139%
22	17.692	2648	2653	2657	rVV	488899	578466	7.85%	1.024%
23	17.928	2687	2693	2696	rBV	6244386	7371057	100.00%	13.052%
24	18.280	2749	2753	2758	rBV2	73839	122496	1.66%	0.217%
25	19.163	2898	2903	2914	rBV	337575	637321	8.65%	1.129%
26	19.280	2917	2923	2926	rVV	2113990	2499692	33.91%	4.426%
27	19.310	2926	2928	2932	rVB	198632	210228	2.85%	0.372%
28	19.569	2969	2972	2977	rBV	168825	173967	2.36%	0.308%
29	19.957	3035	3038	3042	rBV	227154	246507	3.34%	0.436%
30	20.333	3099	3102	3109	rVB	294384	359183	4.87%	0.636%
31	20.422	3113	3117	3121	rBV2	86422	107744	1.46%	0.191%
32	20.563	3138	3141	3153	rVB	149699	351912	4.77%	0.623%
33	20.733	3166	3170	3176	rBV	288433	357567	4.85%	0.633%
34	20.910	3197	3200	3207	rVB	104671	140066	1.90%	0.248%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
Data File : BP001052.D
Acq On : 15 Nov 2019 21:26
Operator : JU
Sample : K5832-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
6-(6-8)

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	20.980	3208	3212	3219	rVV	144893	190228	2.58%	0.337%
36	21.063	3220	3226	3234	rVB	1528938	2209731	29.98%	3.913%
37	21.180	3241	3246	3252	rVB	243547	369373	5.01%	0.654%
38	21.680	3326	3331	3340	rBV	169649	307244	4.17%	0.544%
39	22.268	3426	3431	3440	rVB	87527	166833	2.26%	0.295%
40	23.204	3585	3590	3598	rVB2	57329	123442	1.67%	0.219%

Sum of corrected areas: 56474435

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Acq On : 15 Nov 2019 21:26
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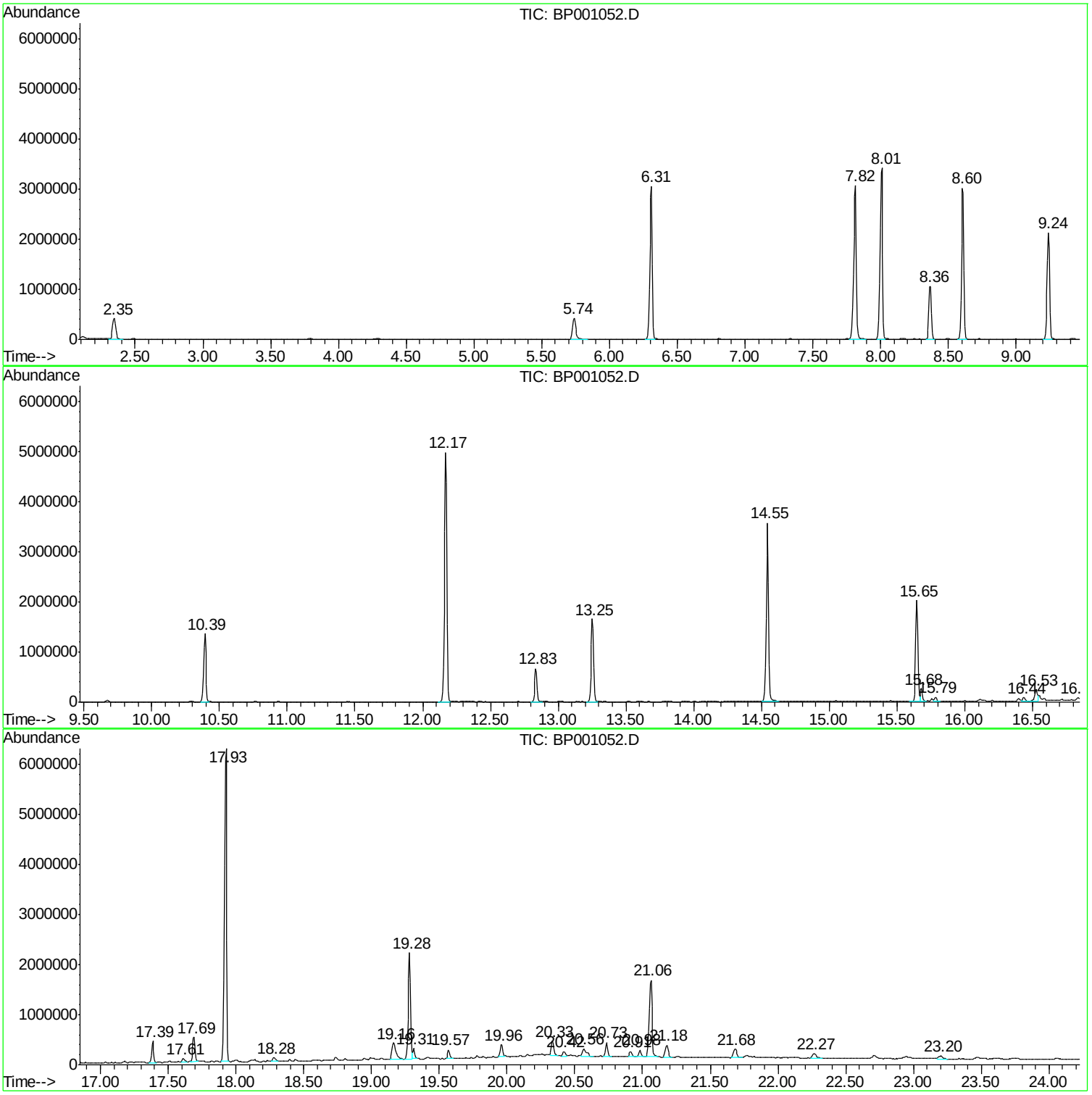
Sample : K5832-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 6-(6-8)

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\BP111519\
Data File : BP001052.D
Acq On : 15 Nov 2019 21:26
Operator : JU
Sample : K5832-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 6-(6-8)

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

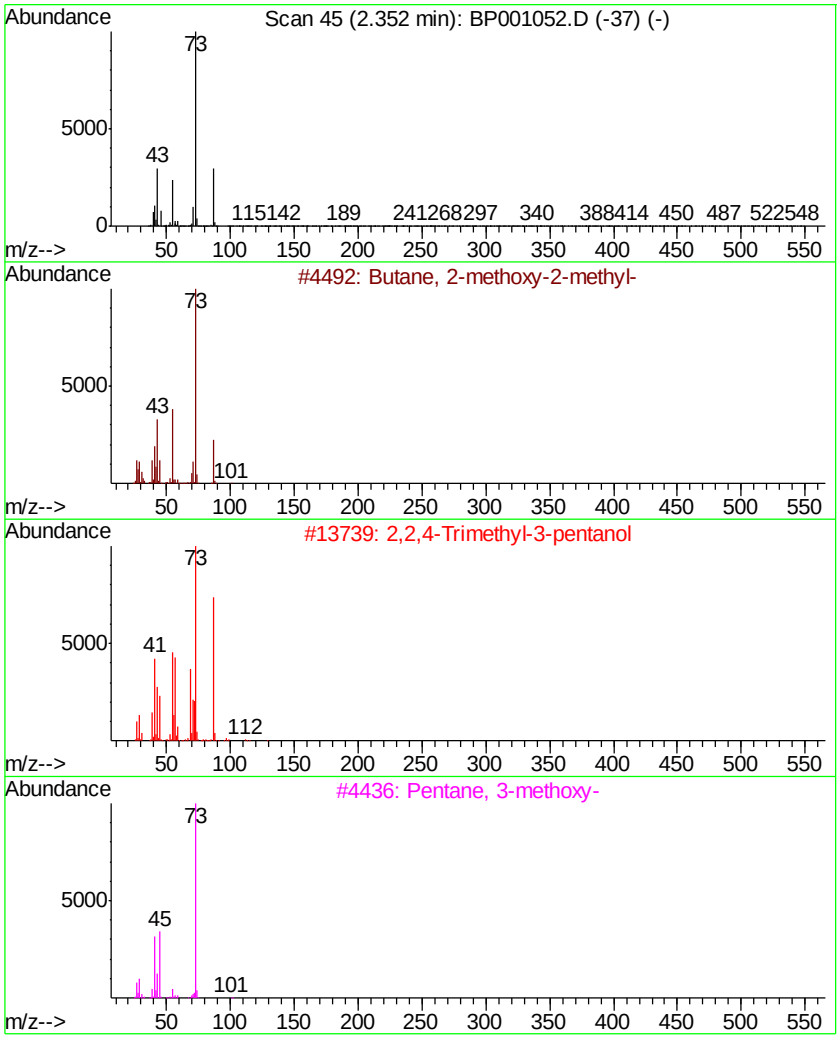
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

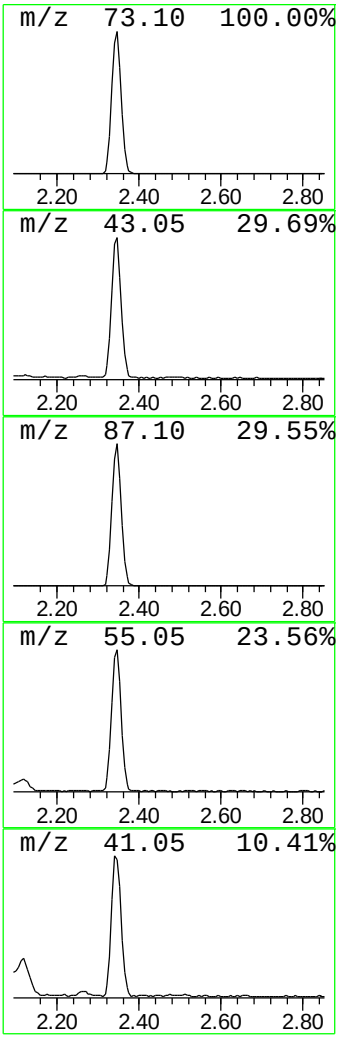
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.35	10.07 ng	634019	1,4-Dichlorobenzene-d4	8.37

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	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
Data File : BP001052.D
Acq On : 15 Nov 2019 21:26
Operator : JU
Sample : K5832-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 6-(6-8)

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

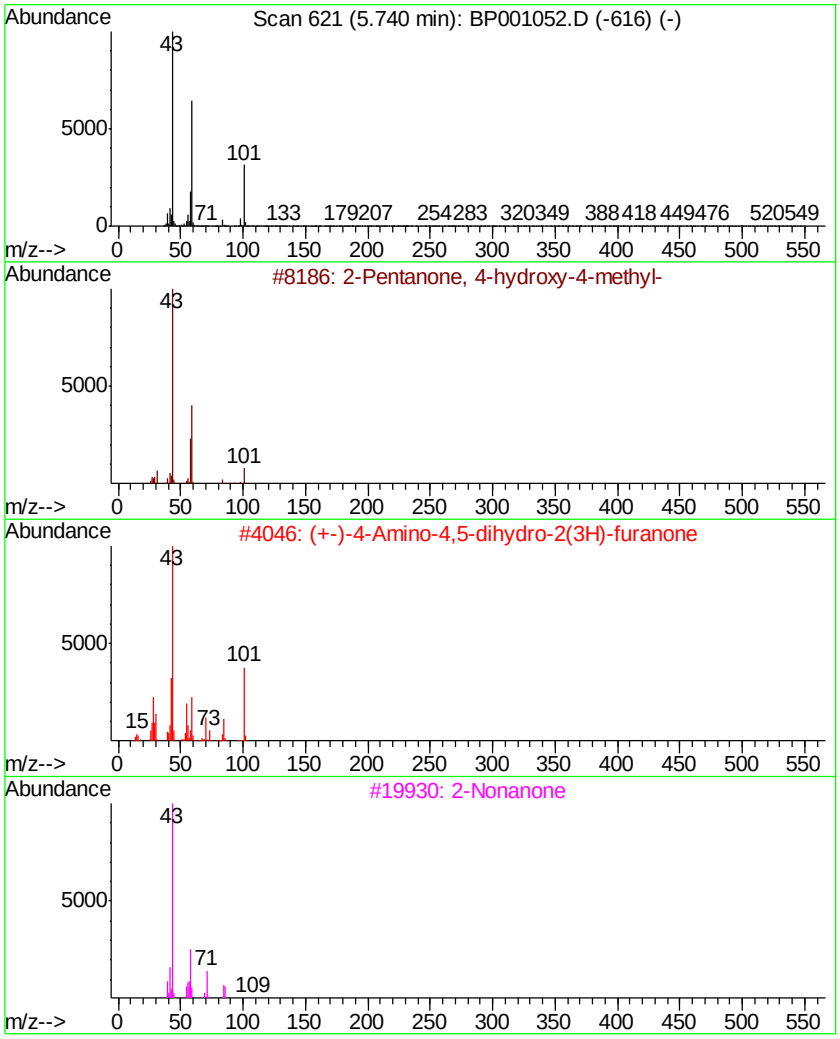
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

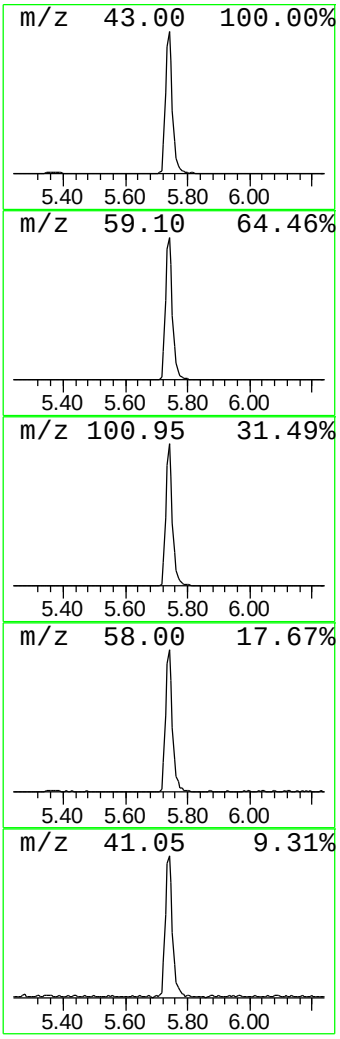
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.74	10.51 ng	661827	1,4-Dichlorobenzene-d4	8.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3	2-Nonanone	142	C9H18O	000821-55-6	12
4	Acetone	58	C3H6O	000067-64-1	10
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
Data File : BP001052.D
Acq On : 15 Nov 2019 21:26
Operator : JU
Sample : K5832-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 6-(6-8)

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

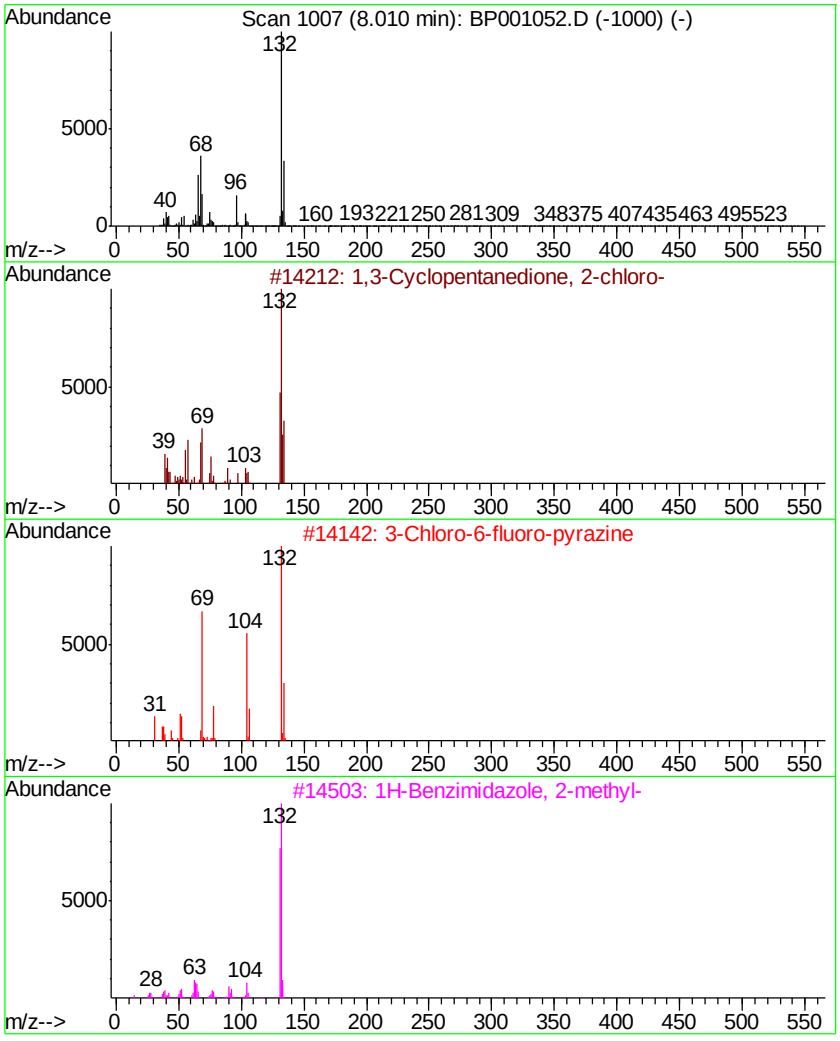
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

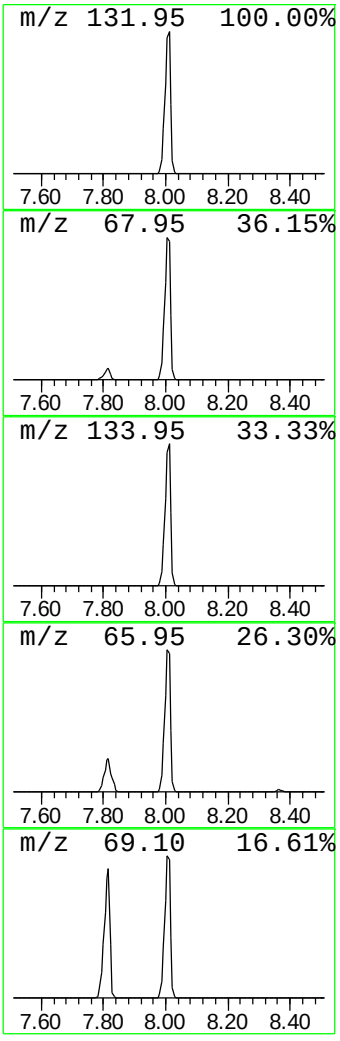
****

Peak Number 3 unknown8.01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.01	70.26 ng	4423940	1,4-Dichlorobenzene-d4	8.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	38
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	27
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
5	5-Aminoindole	132	C8H8N2	005192-03-0	16





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
Data File : BP001052.D
Acq On : 15 Nov 2019 21:26
Operator : JU
Sample : K5832-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 6-(6-8)

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

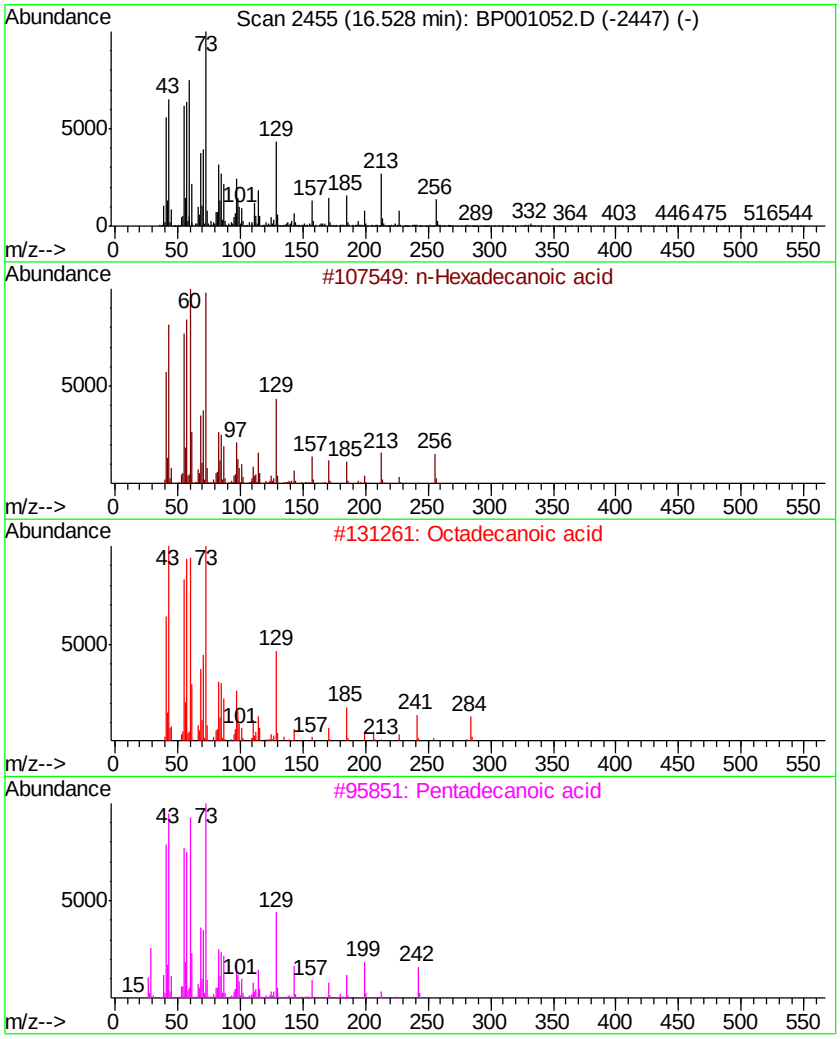
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

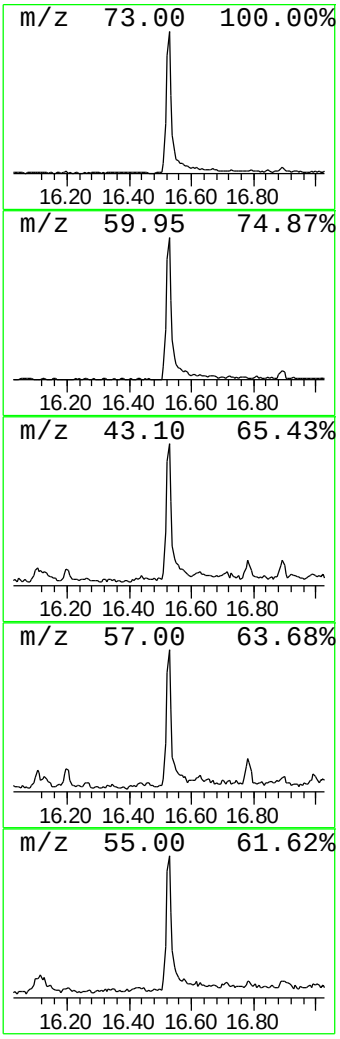
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	2.55 ng	290833	Phenanthrene-d10	15.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	89
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	81





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
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Acq On : 15 Nov 2019 21:26
Operator : JU
Sample : K5832-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 6-(6-8)

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

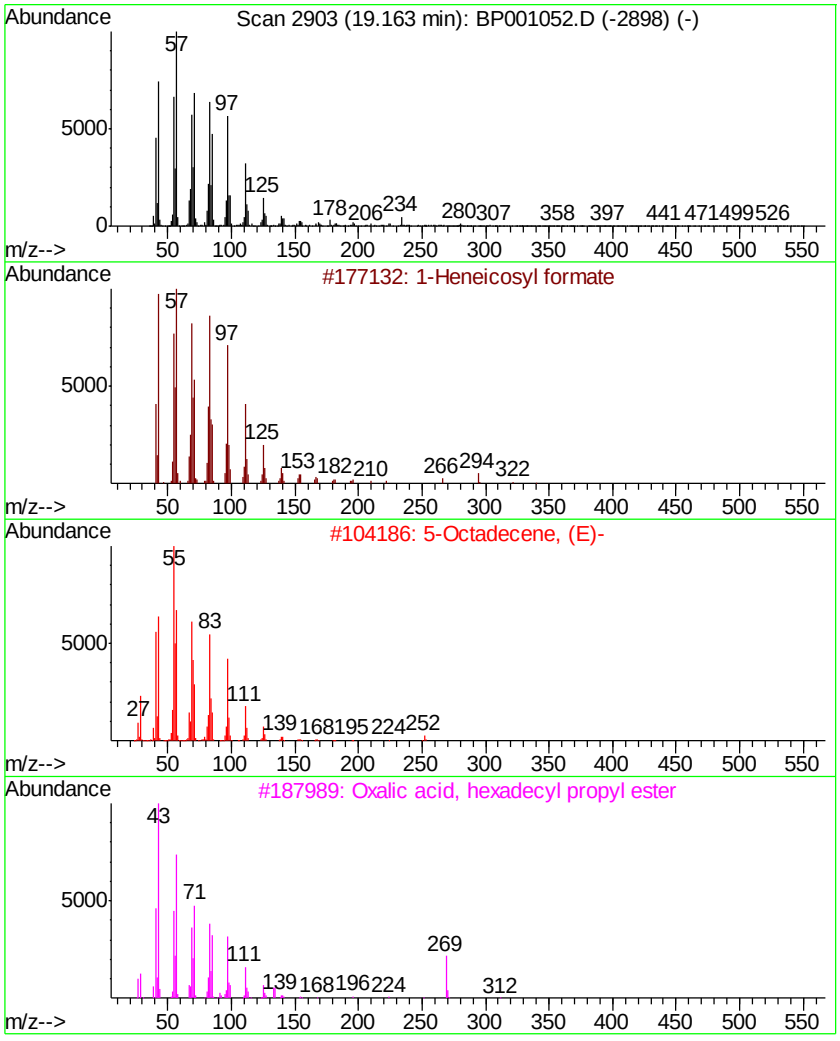
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

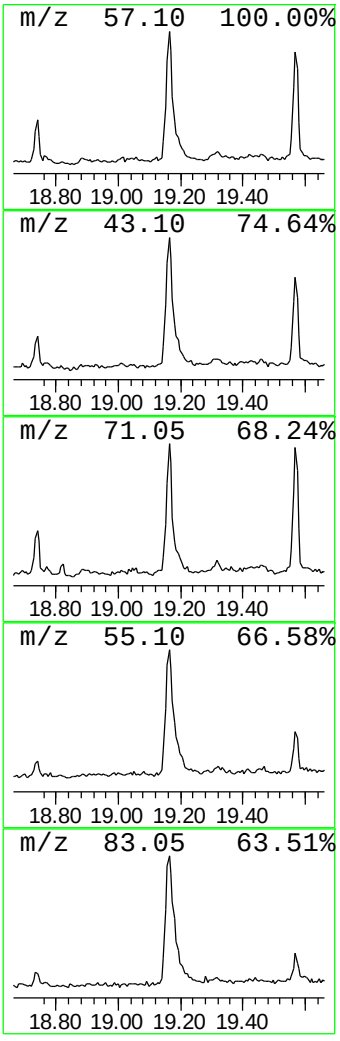
****

Peak Number 6 1-Heneicosyl formate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.16	5.10 ng	637321	Chrysene-d12	19.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	99
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	93
3	Oxalic acid, hexadecyl propyl ester	356	C21H40O4	1000309-26-9	91
4	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	91
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	91





Library Search Compound Report

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Sample : K5832-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 6-(6-8)

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

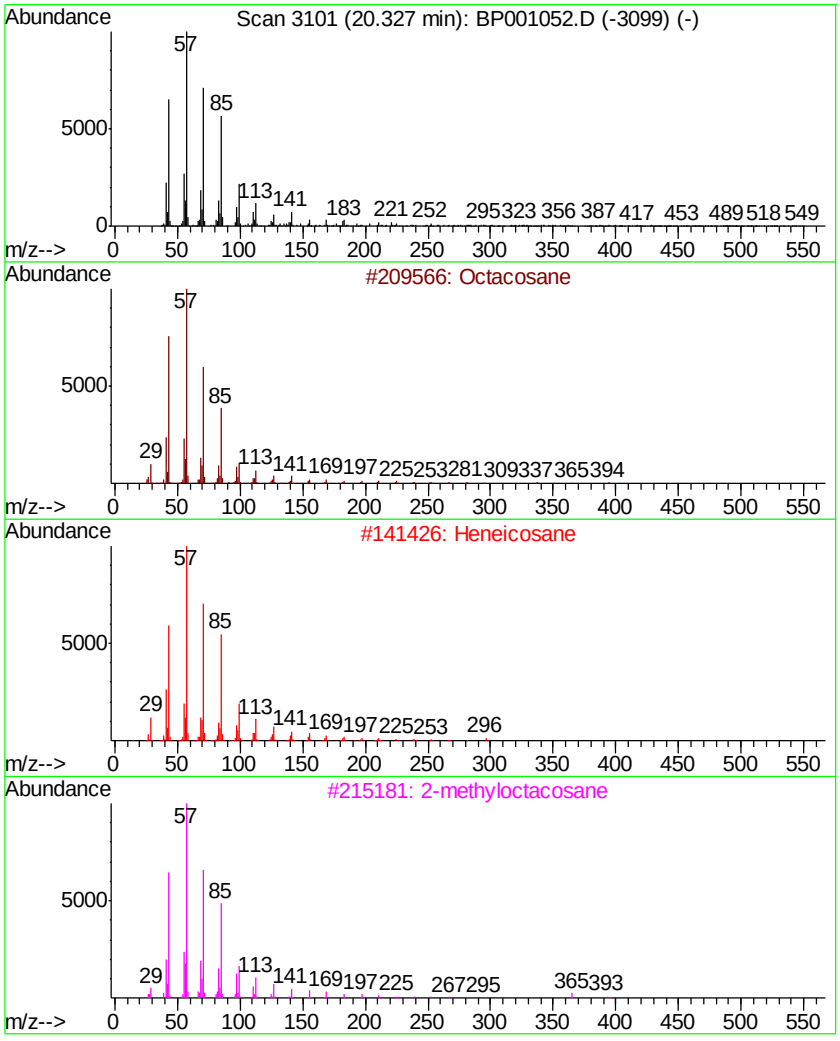
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

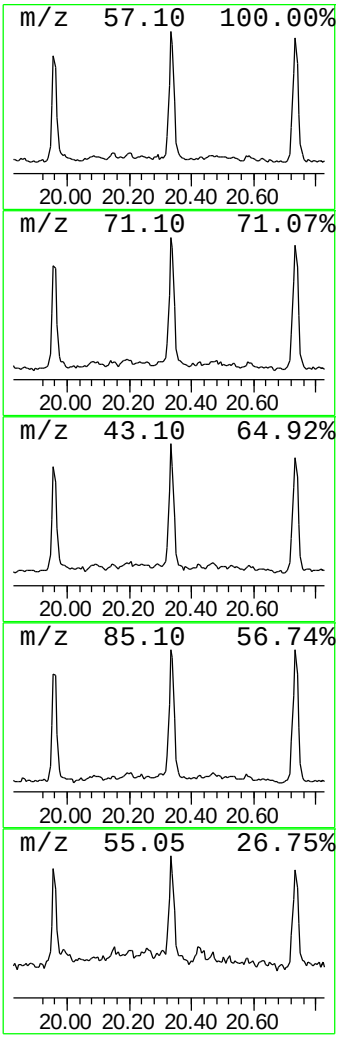
****

Peak Number 7 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.33	3.25 ng	359183	Perylene-d12	21.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Triacontane	422	C30H62	000638-68-6	87





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Acq On : 15 Nov 2019 21:26
Operator : JU
Sample : K5832-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 6-(6-8)

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

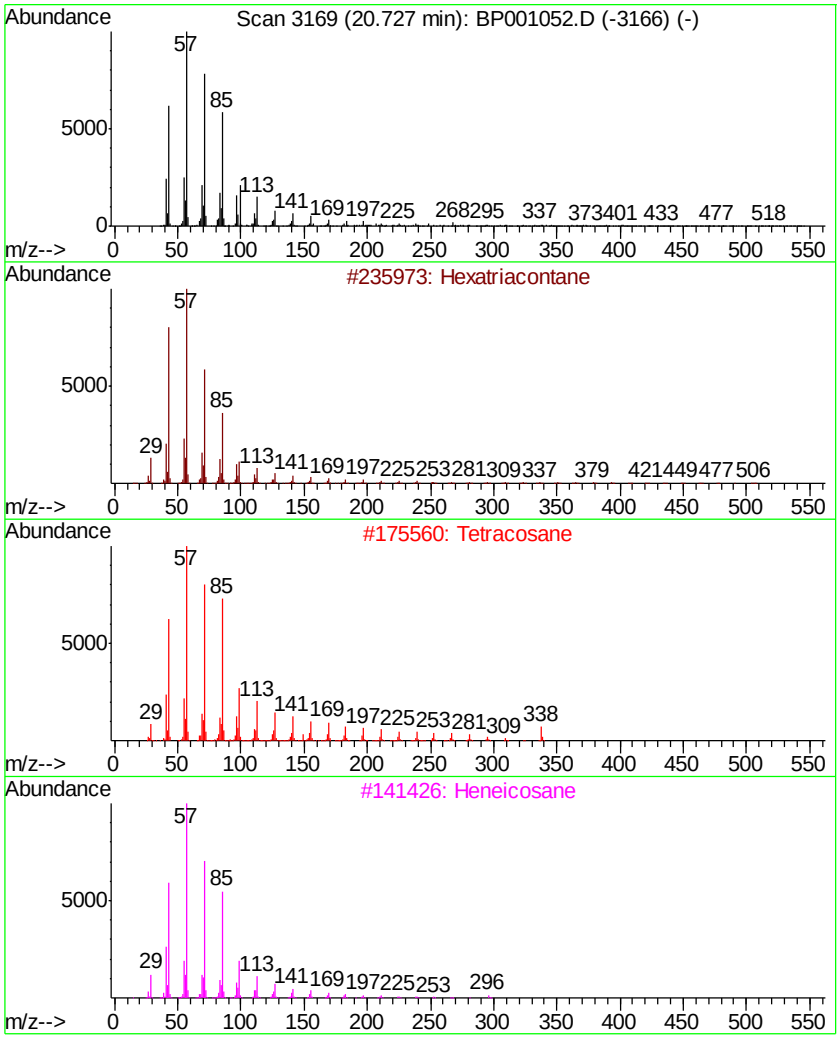
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

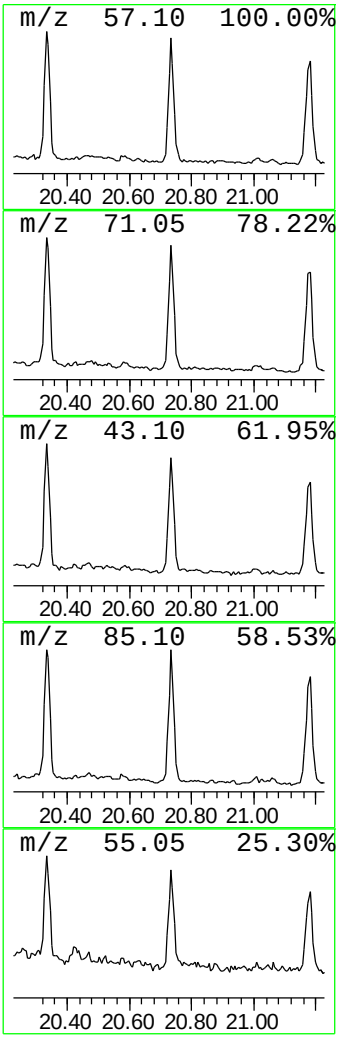
****

Peak Number 8 Hexatriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.73	3.24 ng	357567	Perylene-d12	21.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexatriacontane	507	C36H74	000630-06-8	97
2	Tetracosane	338	C24H50	000646-31-1	97
3	Heneicosane	296	C21H44	000629-94-7	95
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	95
5	Octacosane	394	C28H58	000630-02-4	95





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
Data File : BP001052.D
Acq On : 15 Nov 2019 21:26
Operator : JU
Sample : K5832-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 6-(6-8)

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

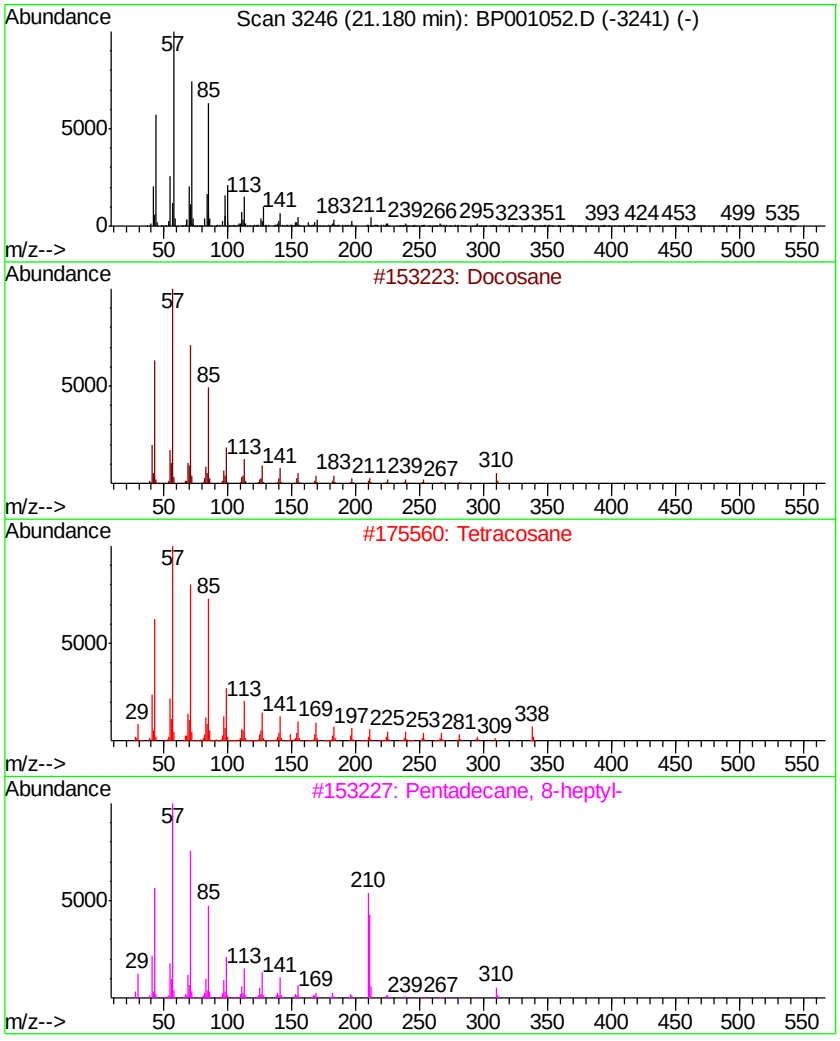
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

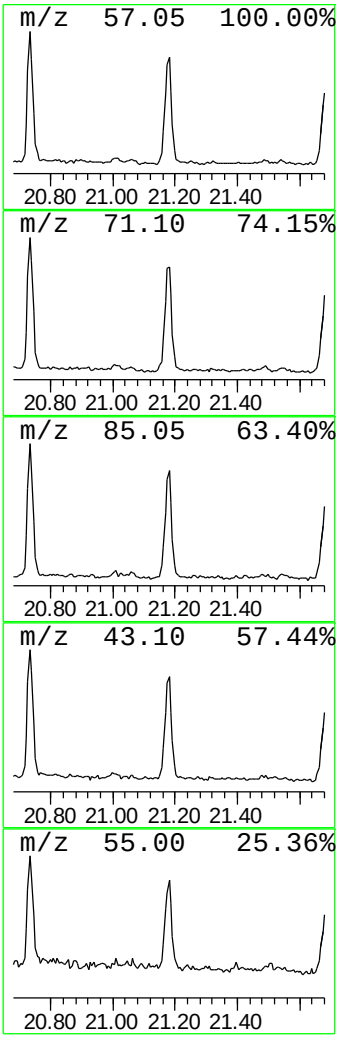
****

Peak Number 9 Docosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.18	3.34 ng	369373	Perylene-d12	21.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	95
2	Tetracosane	338	C24H50	000646-31-1	95
3	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	94
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	94
5	Heneicosane	296	C21H44	000629-94-7	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
Data File : BP001052.D
Acq On : 15 Nov 2019 21:26
Operator : JU
Sample : K5832-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 6-(6-8)

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

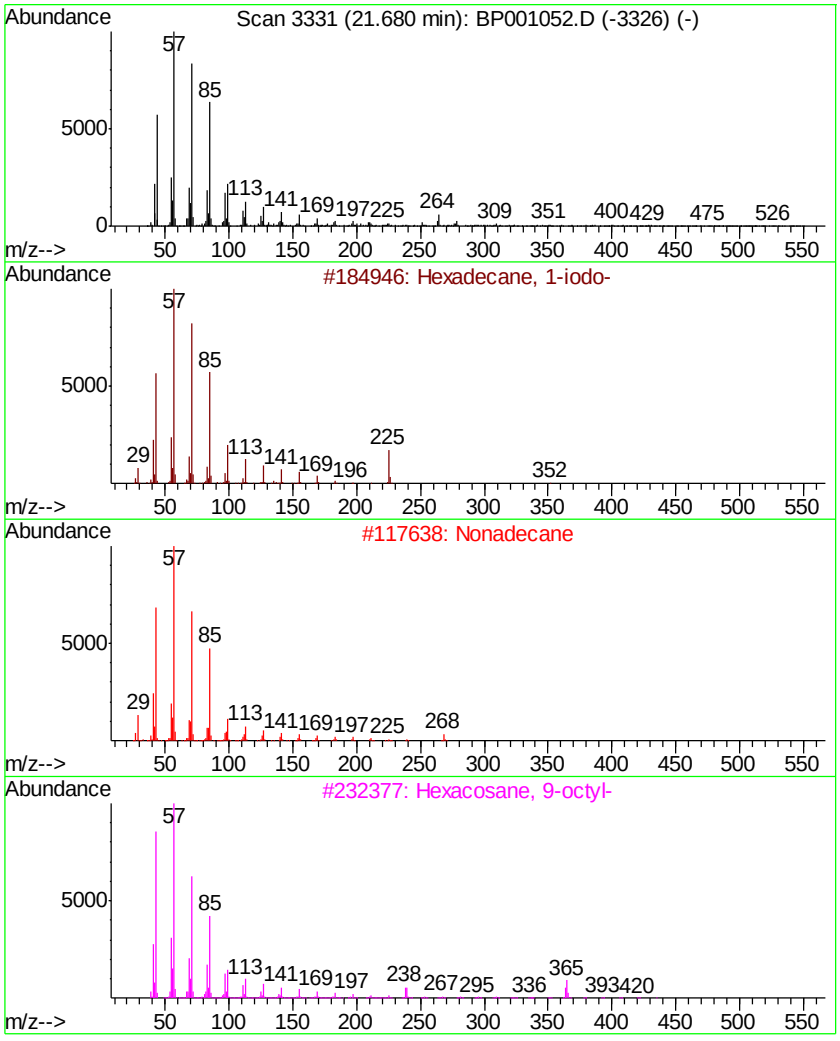
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

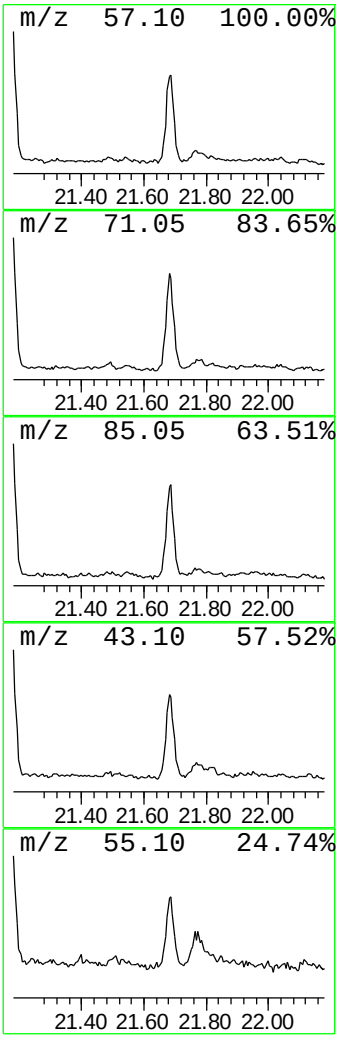
****

Peak Number 10 Hexadecane, 1-iodo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.68	2.78 ng	307244	Perylene-d12	21.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	96
2	Nonadecane	268	C19H40	000629-92-5	93
3	Hexacosane, 9-octyl-	479	C34H70	055429-83-9	91
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP111519\
Data File : BP001052.D
Acq On : 15 Nov 2019 21:26
Operator : JU
Sample : K5832-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
6-(6-8)

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...	2.35	10.1	ng	634019	1	8.37	1259270	20.0
2-Pentanone, 4-hy...	5.74	10.5	ng	661827	1	8.37	1259270	20.0
unknown8.01	8.01	70.3	ng	4423940	1	8.37	1259270	20.0
n-Hexadecanoic acid	16.53	2.5	ng	290833	4	15.65	2284410	20.0
1-Heneicosyl formate	19.16	5.1	ng	637321	5	19.28	2499690	20.0
Octacosane	20.33	3.3	ng	359183	6	21.06	2209730	20.0
Hexatriacontane	20.73	3.2	ng	357567	6	21.06	2209730	20.0
Docosane	21.18	3.3	ng	369373	6	21.06	2209730	20.0
Hexadecane, 1-iodo-	21.68	2.8	ng	307244	6	21.06	2209730	20.0