LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122719\
Data File : BP001477.D
Acq On : 28 Dec 2019 00:47
Operator : JU
Sample : K6438-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DUNR-BF007-01

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-BP121919.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	5.587	590	595	606	rVB	65209	97336	12.06%	1.672%
2	6.198	694	699	713	rBV	352498	468278	58.00%	8.045%
3	7.745	956	962	980	rBV	398204	508033	62.92%	8.728%
4	7.928	987	993	1000	rBV	453393	524262	64.93%	9.007%
5	8.281	1048	1053	1060	rBV	125320	142134	17.60%	2.442%
6	8.522	1088	1094	1105	rVB	351758	420252	52.05%	7.220%
7	9.163	1197	1203	1214	rBV	248646	319834	39.61%	5.495%
8	10.316	1394	1399	1415	rBV	122269	165957	20.56%	2.851%
9	12.098	1696	1702	1719	rBV	489961	619996	76.79%	10.651%
10	12.769	1812	1816	1828	rBV2	8381	15363	1.90%	0.264%
11	13.180	1879	1886	1897	rBV	150961	210309	26.05%	3.613%
12	14.474	2100	2106	2130	rBV	342256	490541	60.76%	8.427%
13	15.574	2288	2293	2306	rBV	181018	236764	29.33%	4.068%
14	16.468	2441	2445	2458	rBV3	19834	30471	3.77%	0.523%
15	17.863	2676	2682	2686	rBV	763095	807377	100.00%	13.871%
16	19.139	2894	2899	2908	rVV6	25262	82641	10.24%	1.420%
17	19.221	2908	2913	2929	rVB	193109	246089	30.48%	4.228%
18	19.504	2958	2961	2965	rBV2	8625	8866	1.10%	0.152%
19	19.862	3010	3022	3023	rBV6	20579	47512	5.88%	0.816%
20	19.898	3025	3028	3035	rVB3	23735	36449	4.51%	0.626%
21	20.274	3088	3092	3097	rVB	15870	18857	2.34%	0.324%
22	20.351	3101	3105	3111	rVB	26559	30033	3.72%	0.516%
23	20.662	3153	3158	3165	rVB	16659	22664	2.81%	0.389%
24	20.986	3207	3213	3226	rVB	146752	214899	26.62%	3.692%
25	21.092	3227	3231	3237	rVB3	14529	21453	2.66%	0.369%
26	21.586	3310	3315	3319	rVB2	12507	20135	2.49%	0.346%
27	22.151	3407	3411	3419	rVB6	7537	14303	1.77%	0.246%

Sum of corrected areas: 5820808

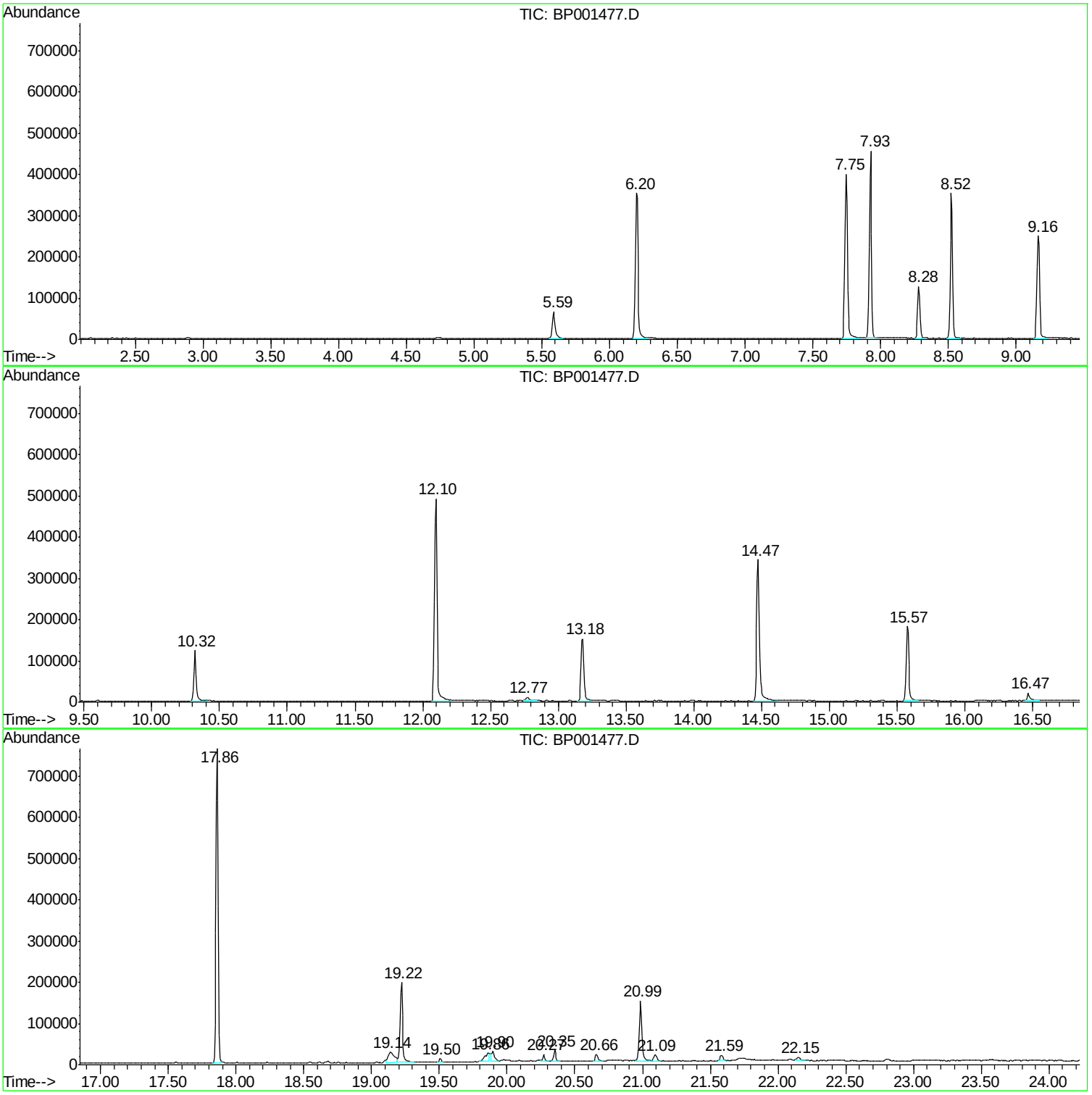
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122719\
Data File : BP001477.D
Acq On : 28 Dec 2019 00:47
Operator : JU
Sample : K6438-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DUNR-BF007-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.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\BP122719\
Data File : BP001477.D
Acq On : 28 Dec 2019 00:47
Operator : JU
Sample : K6438-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DUNR-BF007-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

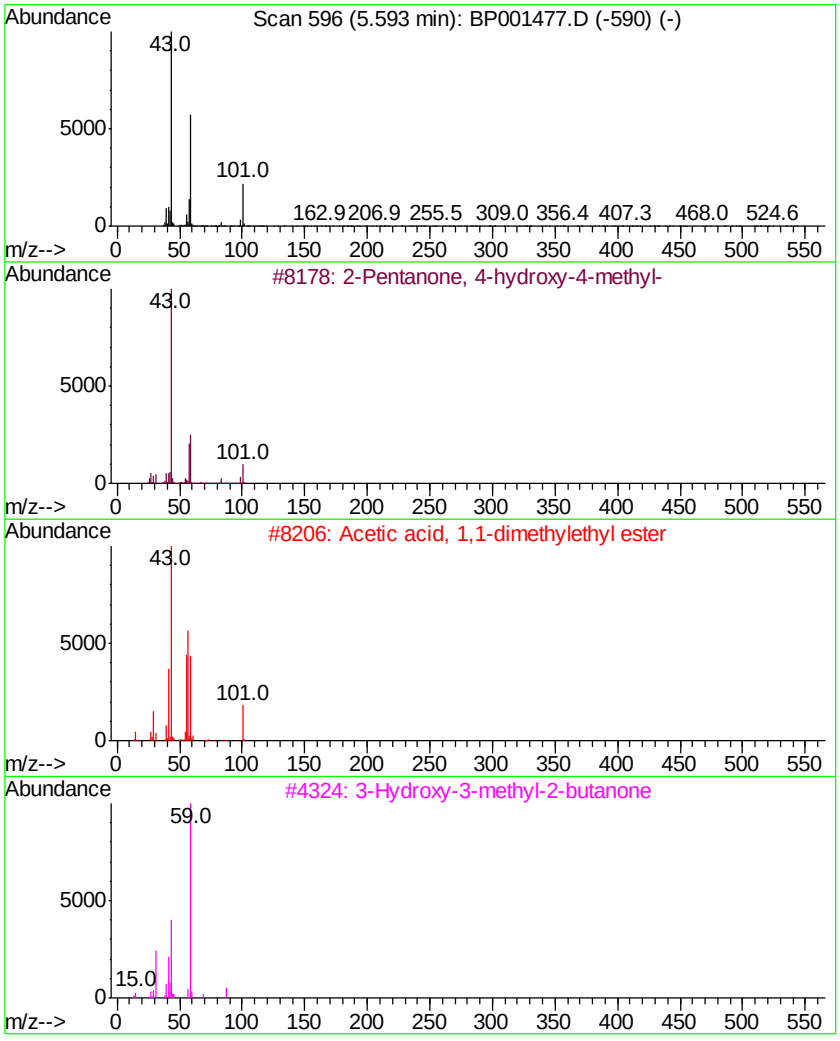
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

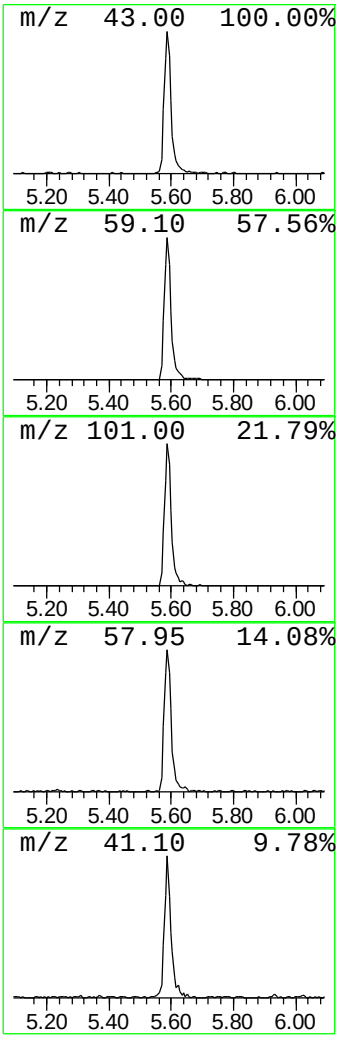
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.59	13.70 ng	97336	1,4-Dichlorobenzene-d4	8.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
5	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	17





Library Search Compound Report

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Data File : BP001477.D
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Operator : JU
Sample : K6438-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DUNR-BF007-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.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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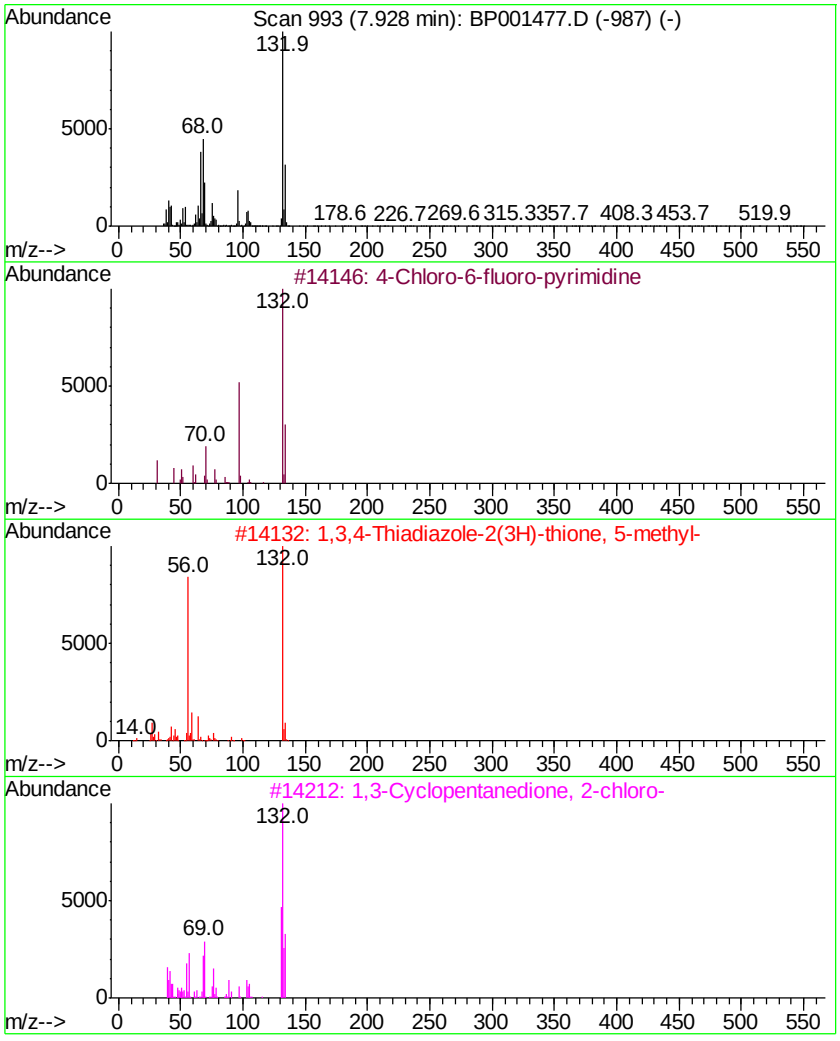
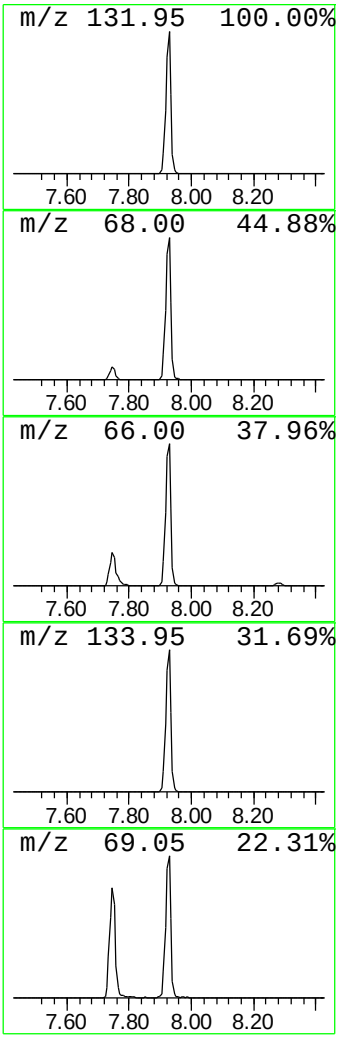
Peak Number 2 unknown7.93 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.93	73.77 ng	524262	1,4-Dichlorobenzene-d4	8.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	27
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
4	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	22
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	22





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122719\
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Operator : JU
Sample : K6438-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DUNR-BF007-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.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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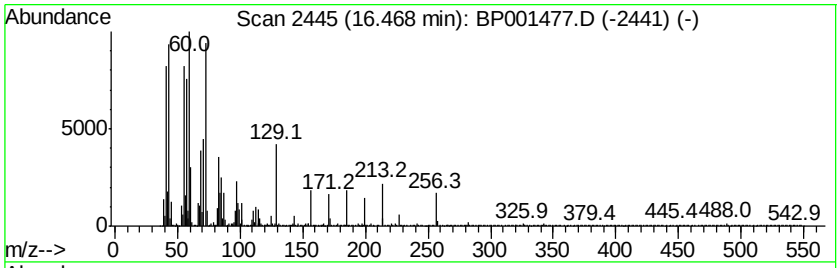
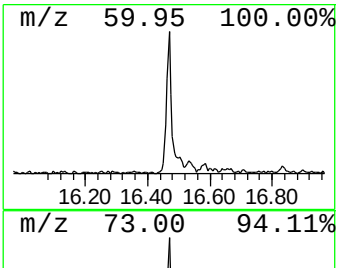
Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.47	2.57 ng	30471	Phenanthrene-d10	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Tridecanoic acid	214	C13H26O2	000638-53-9	59
4	Octadecanoic acid	284	C18H36O2	000057-11-4	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122719\
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Acq On : 28 Dec 2019 00:47
Operator : JU
Sample : K6438-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DUNR-BF007-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

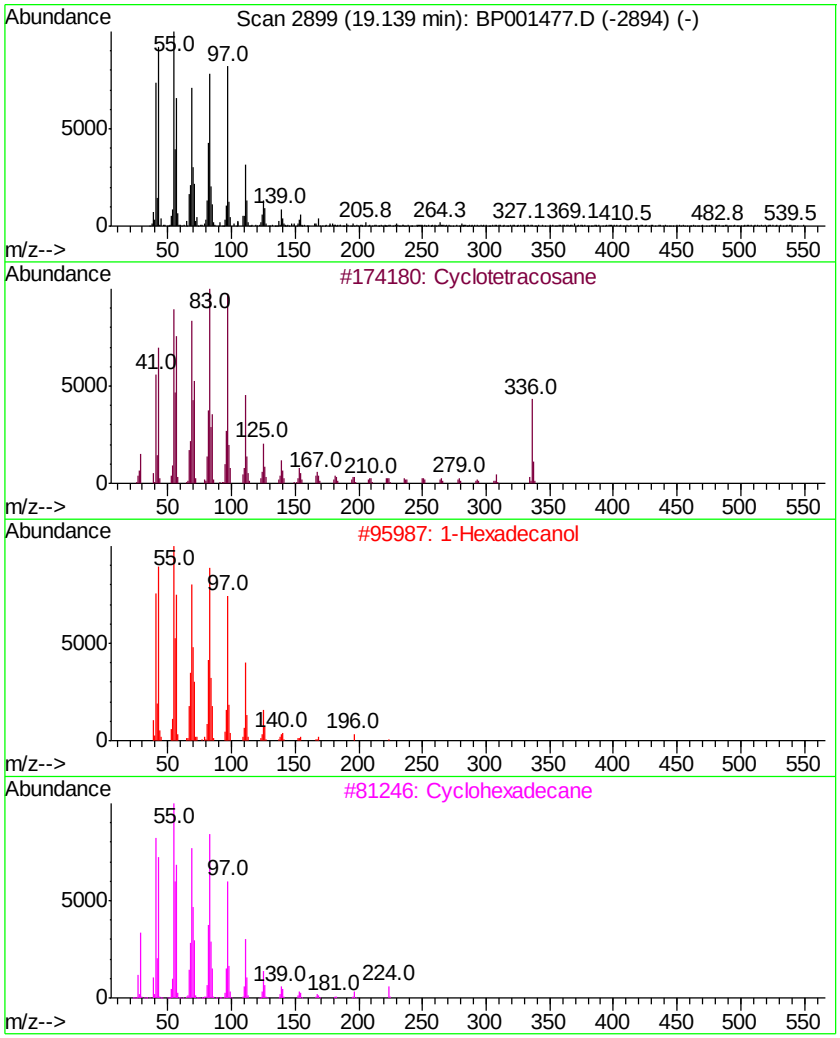
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

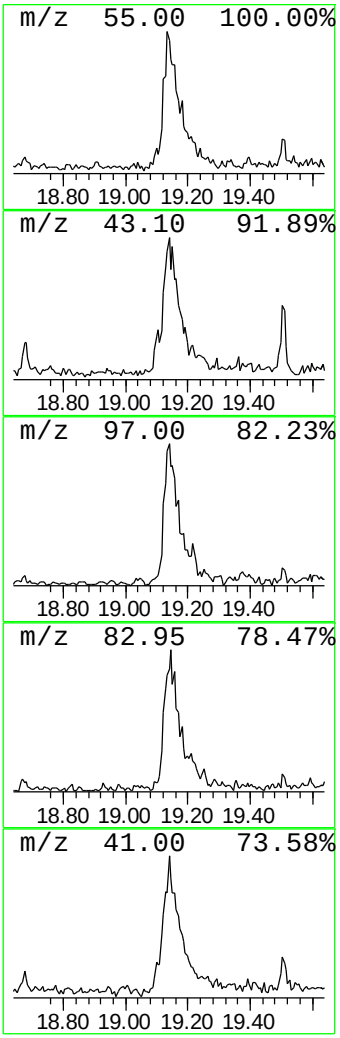
****

Peak Number 5 Cyclotetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.14	6.72 ng	82641	Chrysene-d12	19.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	90
2	1-Hexadecanol	242	C16H34O	036653-82-4	76
3	Cyclohexadecane	224	C16H32	000295-65-8	68
4	2-Methyl-2-docosene	322	C23H46	1000131-16-9	64
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122719\
Data File : BP001477.D
Acq On : 28 Dec 2019 00:47
Operator : JU
Sample : K6438-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DUNR-BF007-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

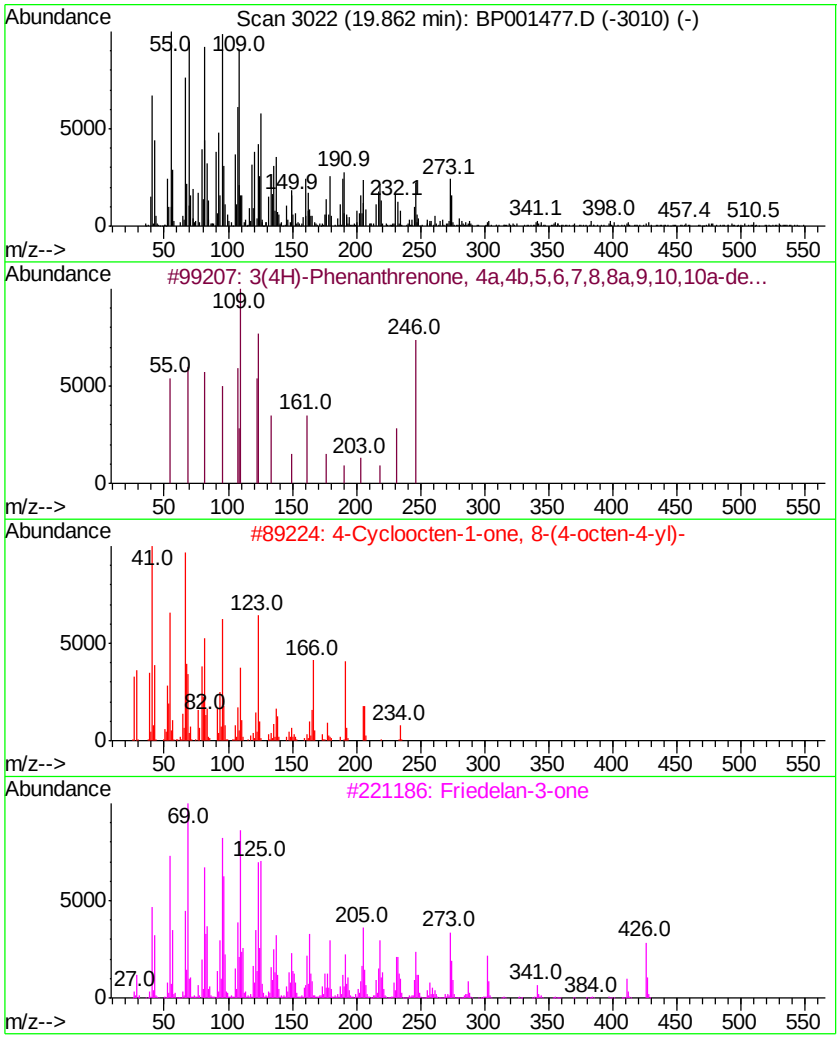
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

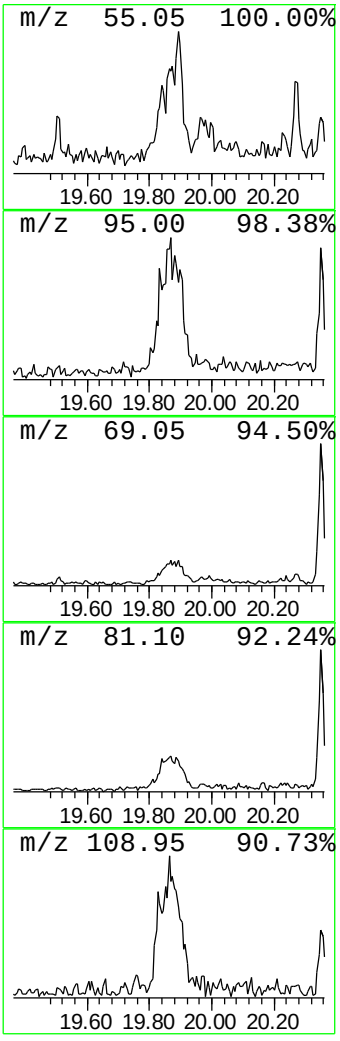
****

Peak Number 6 3(4H)-Phenanthrenone, 4a,4b... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.86	3.86 ng	47512	Chrysene-d12	19.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3(4H)-Phenanthrenone, 4a,4b,5,6,...	246	C17H26O	057684-12-5	83
2	4-Cycloocten-1-one, 8-(4-octen-4...	234	C16H26O	1000152-01-9	59
3	Friedelan-3-one	426	C30H50O	000559-74-0	55
4	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	53
5	Caparratriene	206	C15H26	1000374-08-7	52





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ClientSampleId : DUNR-BF007-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

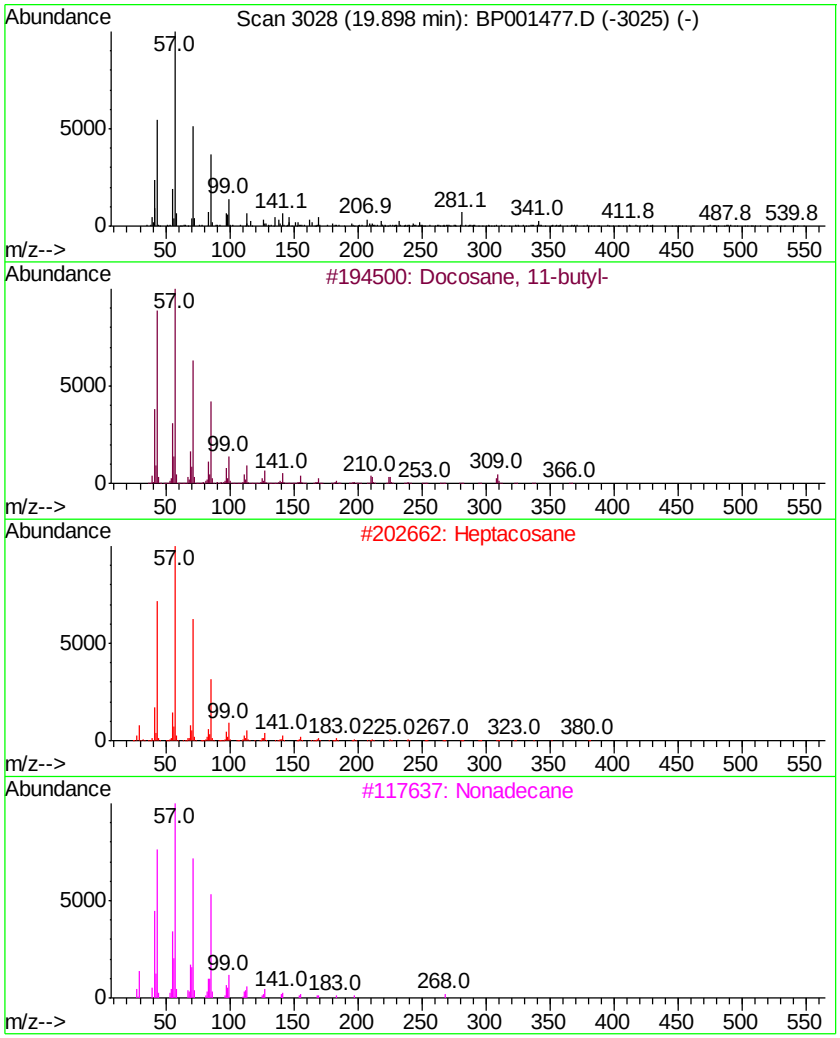
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

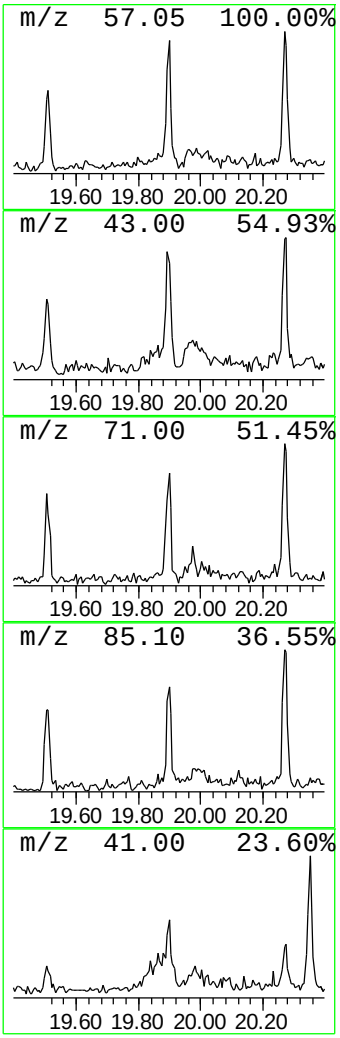
****

Peak Number 7 Docosane, 11-butyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.90	2.96 ng	36449	Chrysene-d12	19.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-	366	C26H54	013475-76-8	76
2	Heptacosane	380	C27H56	000593-49-7	72
3	Nonadecane	268	C19H40	000629-92-5	72
4	Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	64
5	Heptadecane	240	C17H36	000629-78-7	64





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Misc :
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Instrument : BNA_P
ClientSampleId : DUNR-BF007-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

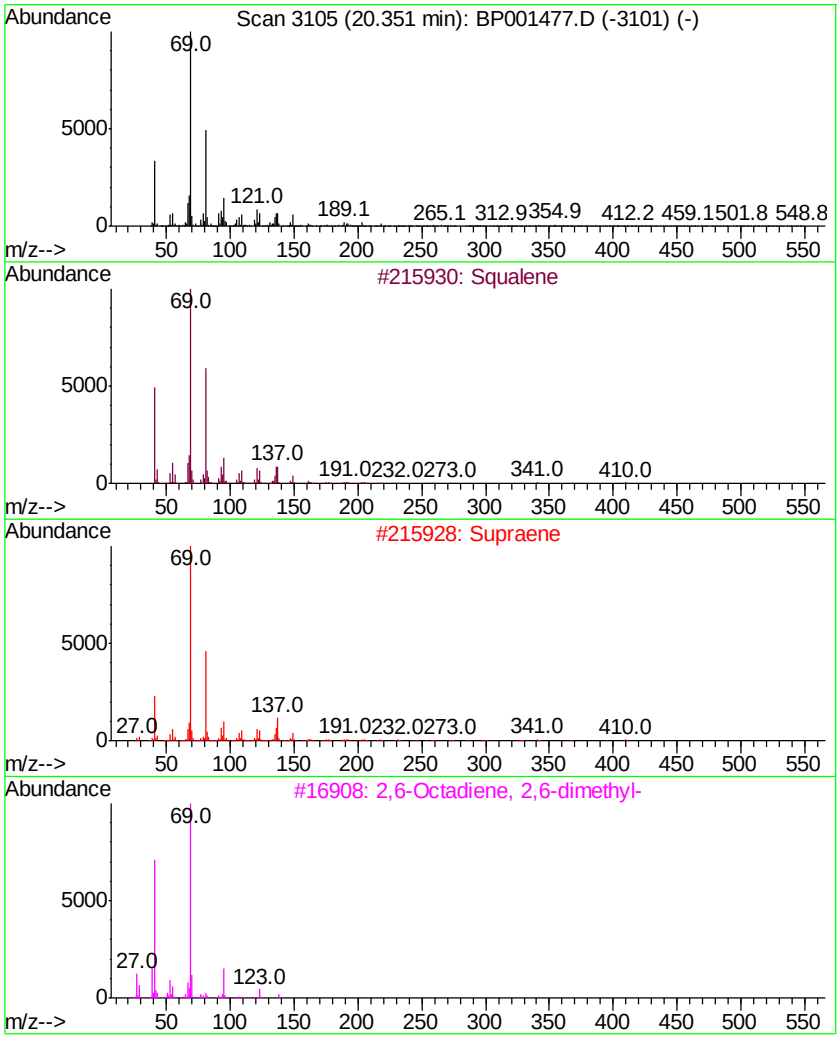
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

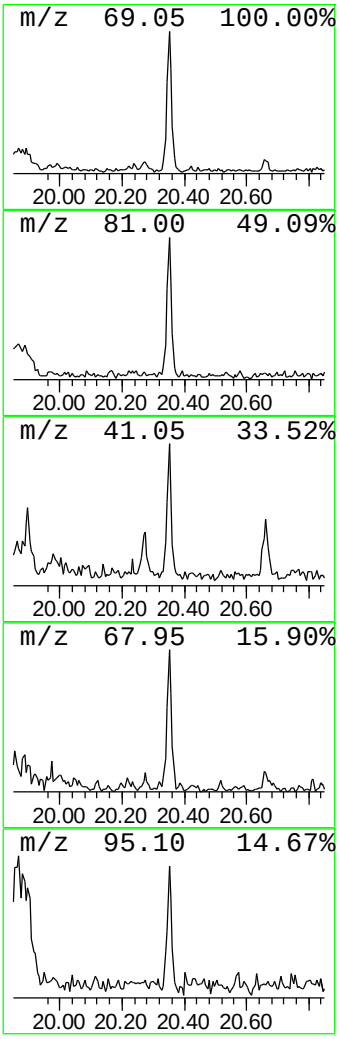
****

Peak Number 8 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.35	2.80 ng	30033	Perylene-d12	20.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	90
2	Supraene	410	C30H50	007683-64-9	87
3	2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	59
4	Trideca-1,7,11-triene-1,1-dicarb...	270	C18H26N2	1000161-46-0	53
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	53





Library Search Compound Report

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TIC Library : C:\DATABASE\NIST11.L
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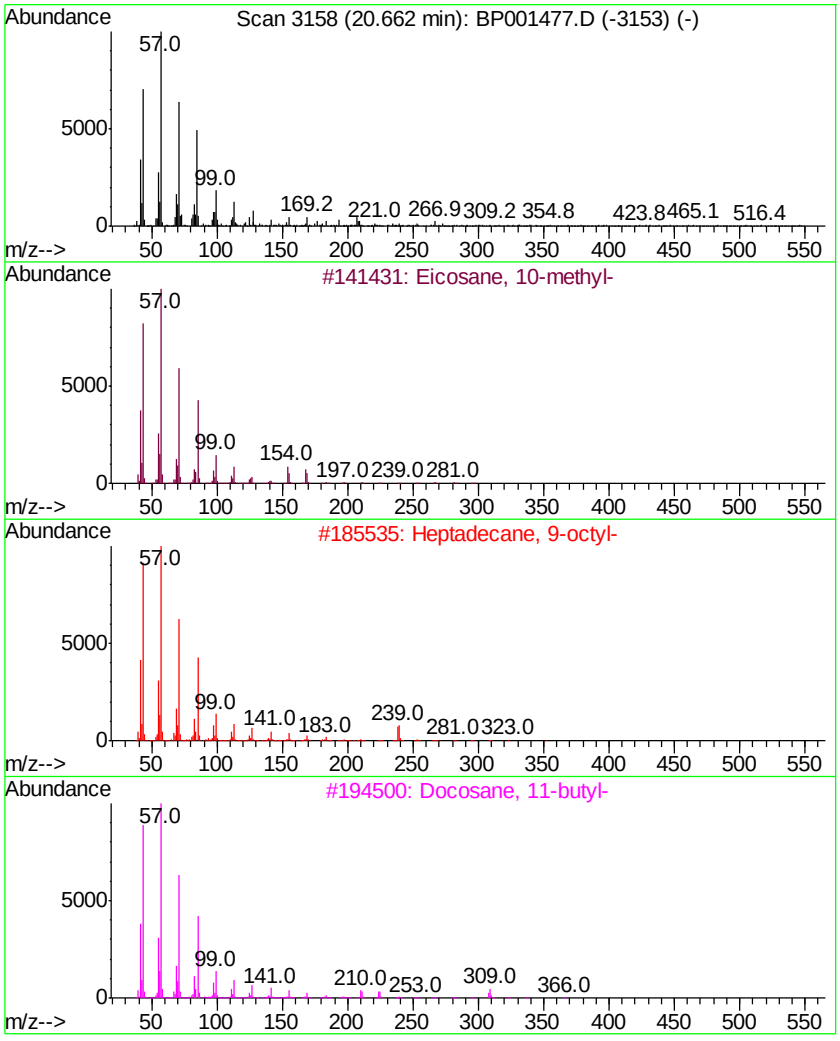
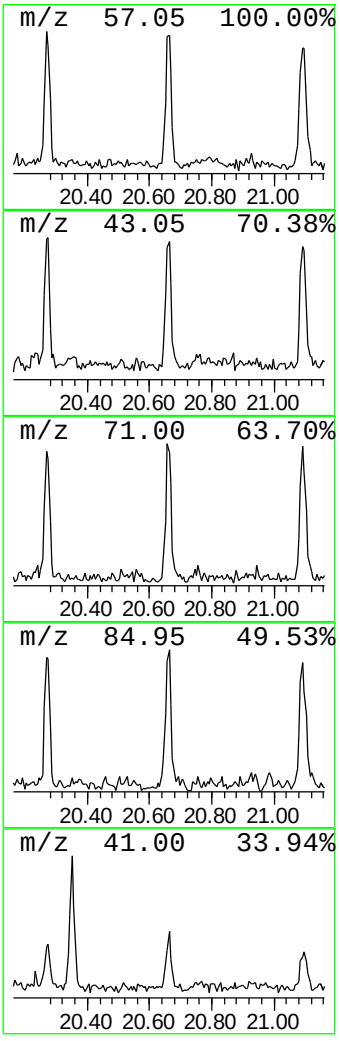
Peak Number 9 Eicosane, 10-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.66	2.11 ng	22664	Perylene-d12	20.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	95
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	90
4	Tridecane, 7-propyl-	226	C16H34	055045-09-5	90
5	Tridecane, 6-propyl-	226	C16H34	055045-10-8	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP122719\
Data File : BP001477.D
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ClientSampleId : DUNR-BF007-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.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
2-Pentanone, 4-hy...	5.59	13.7	ng	97336	1	8.28	142134	20.0
unknown7.93	7.93	73.8	ng	524262	1	8.28	142134	20.0
n-Hexadecanoic acid	16.47	2.6	ng	30471	4	15.57	236764	20.0
Cyclotetracosane	19.14	6.7	ng	82641	5	19.22	246089	20.0
3(4H)-Phenanthren...	19.86	3.9	ng	47512	5	19.22	246089	20.0
Docosane, 11-butyl-	19.90	3.0	ng	36449	5	19.22	246089	20.0
Squalene	20.35	2.8	ng	30033	6	20.99	214899	20.0
Eicosane, 10-methyl-	20.66	2.1	ng	22664	6	20.99	214899	20.0